PB84-189257

Intermediate-Range Grid Model and User's Guide for Atmospheric Sulfur Dioxide and Sulfate Concentrations and Depositions Wisconsin Power Plant Impact Study

Wisconsin Univ.-Madison

Prepared for

Environmental Research Lab.-Duluth, MN

May 84

U.S. Department of Commerce
National Technical Information Service
NTIS

PB84-189257

EPA-600/3-84-061
May 1984

INTERMEDIATE-RANGE GRID MODEL AND USER'S GUIDE FOR ATMOSPHERIC SULFUR DIOXIDE AND SULFATE CONCENTRATIONS AND DEPOSITIONS

Wisconsin Power Plant Impact Study

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Grant No. R806878-01-5

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This study was conducted in cooperation with

Wisconsin Power and Light Company
Madison Gas and Electric Company,
Wisconsin Public Service Corporation,
Wisconsin Public Service Commission,
and Wisconsin Department of Natural Resources

ENVIRONMENTAL RESEARCH LABORATORY-DULUTH
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
DULUTH, MINNESOTA 55804

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NATIONAL TECHNICAL
INFORMATION SERVICE
U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/3-84-061

2.

3. RECIPIENT'S ACCESSION NO. PB8 4 189257

4. TITLE AND SUBTITLE
INTERMEDIATE-RANGE GRID MODEL AND USER'S GUIDE FOR
ATMOSPHERIC SULFUR DIOXIDE AND SULFATE
CONCENTRATIONS AND DEPOSITIONS

5. REPORT DATE May 1984

6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)
Kenneth E. Wilkening and Kenneth W. Ragland

8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Department of Mechanical Engineering
University of Wisconsin-Madison
Madison, WI 53706

10. PROGRAM ELEMENT NO.

11. CONTRACT/GRANT NO. R80-3971

12. SPONSORING AGENCY NAME AND ADDRESS
Environmental Research Laboratory
6201 Congdon Blvd.
U.S. Environmental Protection Agency
Duluth, MN 61801

13. TYPE OF REPORT AND PERIOD COVERED

14. SPONSORING AGENCY CODE EPA/600/03

15. SUPPLEMENTARY NOTES
101 pages; 22 figures; 9 tables; 2 appendices

16. ABSTRACT

The UWATM-SOX computer model was developed to address the acid rain problem on a mesoscale. It predicts sulfur dioxide (SO_2) and sulfate (SO_4) ambient air concentrations and ground level dry and wet (rain or snow) depositions given certain emission and meteorological input data. It is a time-dependent, cell-type model which numerically solves coupled SO_2 and SO_4 conservation and mass equations described in an exterior frame of reference for a dilute species in the atmospheric boundary layer. Significant features of the model include: Handling arbitrary wind directions; inputting hourly meteorological data; fully computerized processing of meteorological tapes obtained from the National Climate Center; simulataneous handling of point, line, and area sources; accounting for the lofting condition of point source plumes; describing the atmospheric boundary layer by vertically variable but horizontally uniform wind and diffusivity profiles; handling dry deposition by means of a deposition velocity which accounts for terrain and net condition; and handling wet deposition by means of a non-linear cold cloud precipitation model developed by Battelle Pacific Northwest Labs. The model is written in ASCII Fortran and has been applied to the Rainy Lake Watershed in northern Minnesota and southern Ontario. A 1-yr simulation with an 11 x 13 x 6 cell structure and hourly meteorological data changes required 50K core space and took 6 h of computer up (CPU) time.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT
Release to Public

19. SECURITY CLASS (This Report) Unclassified

20. SECURITY CLASS (This page) Unclassified

21. NO. OF PAGES 114

22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

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FOREWORD

The U.S. Environmental Protection Agency (EPA) was designed to coordinate our country's efforts toward protecting and improving the environment. This extremely complex task requires continuous research in a multitude of scientific and technical areas. Such research is necessary to monitor changes in the environment, to discover relationships within that environment, to determine health standards, and to eliminate potentially hazardous effects.

One project, which the EPA is supporting through its Environmental Research Laboratory in Duluth, Minnesota, is the study "The Impacts of Coal-Fired Power Plants on the Environment." This interdisciplinary study, centered mainly around the Columbia Generating Station near Portage Wis., involves investigators and experiments from many academic departments at the University of Wisconsin and is being carried out by the Environmental Monitoring and Data Acquisition Group of the Institute for Environmental Studies at the University of Wisconsin-Madison. Several utilities and state agencies are cooperating in the study: Wisconsin Power and Light Company, Madison Gas and Electric Company, Wisconsin Public Service Corporation, Wisconsin Public Service Commission, and Wisconsin Department of Natural Resources.

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ABSTRACT

The UWATM-SOX computer model was developed to address the acid rain problem on a mesoscale. It predicts sulfur dioxide (SO_2) and sulfate (SO_4) ambient air concentrations and ground level dry and wet (rain or snow) depositions given certain emission and meteorological input data. It is a time-dependent, cell-type model which numerically solves coupled SO_2 and SO_4 conservation and mass equations described in an exterior frame of reference for a dilute species in the atmospheric boundary layer. Significant features of the model include: Handling arbitrary wind directions; inputting hourly meteorological data; fully computerized processing of meteorological tapes obtained from the National Climate Center; simultaneous handling of point, line, and area sources; accounting for the lofting condition of point source plumes; describing the atmospheric boundary layer by vertically variable but horizontally uniform wind and diffusivity profiles; handling dry deposition by means of a deposition velocity which accounts for terrain and net condition; and handling wet deposition by means of a non-linear cold cloud precipitation model developed by Battelle Pacific Northwest Labs. The model is written in ASCII Fortran and has been applied to the Rainy Lake Watershed in northern Minnesota and southern Ontario. A 1-yr simulation with a 11 x 13 x 6 cell structure and hourly meteorological data changes required 50K core space and took 6 hours of computer up (CPU) time.

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ACKNOWLEDGEMENTS

The University of Wisconsin-Madison Air Quality Modeling Group wishes to acknowledge the Environmental Protection Agency for funding the project of which this user's guide is one small product. (Grant no. CR806878-01-5, "Coal-Fired Steam Plants: Human and Environmental Exposure to Air and Water Pollutants").

We also wish to acknowledge and thank Jane Lewis for her excellent typing and Susan Halverson for her excellent graphics work.

SECTION 1

INTRODUCTION

The University of Wisconsin Atmospheric SO_2/SO_4 Computer Model (UWATM-SOX) addresses one aspect of air pollution known as the "Sulfur Problem," which includes the phenomenon popularly known as "acid rain." The model predicts sulfur dioxide (SO_2) and sulfate (SO_4) ambient air concentrations and ground level depositions, dry and wet (rain or snow), given certain emissions and meteorological input data.

Work on advanced air pollution computer models has been going on at the University of Wisconsin-Madison for 10 yr (since 1971) under the direction of Prof. Kenneth W. Ragland. Models of progressive flexibility and capability have been developed and applied to the Madison, WI area (Ragland et al. 1975), to southeastern Wisconsin as part a federally required air quality maintenance plan (Southeastern Wisconsin Regional Planning Commission 1980), to the Columbia (Portage, WI) Power Plant as part of an EPA funded power plant siting study (U.S. Environmental Protection Agency 1980a), and to the Boundary Waters Canoe Area (BWCA) in Northern Minnesota as part of an ecological impact study particularly of the effects of acid rain (U.S. Environmental Protection Agency 1980b). Other related publications and documents include: (Ragland 1973, 1974; Ragland and Dennis 1975; Ragland and Pierce 1975). The model discussed in this guide is the most advanced currently developed.

For a model to rationally approach the atmospheric sulfur problem it must address the following aspects.

1. SO_2 transport and dispersion
2. Chemical transformation of SO_2 to SO_4
3. SO_4 transport and dispersion
4. SO_2, SO_4 dry deposition
5. SO_2, SO_4 wet deposition.

The UWATM-SOX model accounts for all these aspects in as sophisticated a manner as is presently possible given computer time and cost, data base and state-of-the-art research limitations. The model is designed to be a research and a policy-oriented tool.

This User's Guide outlines the model with the purpose of:

1. Acquainting the user with the underlying theory and methodology
2. Showing the user how to execute the programs
3. Demonstrating the output from the model

The method of explanation in this guide will be:

First, to examine the model in a general fashion--
Sections II. Summary of Model Features
III. Overview of Modeling Operation

Second, to discuss the major input data in--
Sections IV. Emissions Data-Base
V. Meteorological Data-Base

Third, to briefly examine the theory in--
Sections VI. Atmospheric Dispersion--Equations and Simulation
VII. Wind and Diffusivity Profiles
VIII. Dry and Wet Deposition Schemes
IX. SO_2/SO_4 Chemistry
X. Point Sources: Plume Rise and Lofting

Fourth, to present the methods of program operation in--
Sections XI. Computer Techniques
XII. Program Preparation
XIII. Program Execution

Fifth, to discuss the model output and its manipulation in--
Section XIV. Output Analysis

SECTION 2

SUMMARY OF MODEL FEATURES

The UWATM-SOX model is a time-dependent, cell-type model. The heart of it is the numerical solution of coupled SO_2 and SO_4 conservation of mass equations described in an Eulerian (fixed) frame of reference for a dilute species in the atmospheric boundary layer. Included are the processes of wind transport, turbulent diffusion, chemical reactions, source input and dry and wet deposition. The numerical solution is a first-order fully implicit scheme.

The model inputs emissions once at the beginning of the simulation and new meteorological data every hour. It performs calculations every 20 min within an hour. (The time-step is variable and can easily be altered if necessary.) As long as data is available any time period for simulation can be chosen. The model has been run for time periods up to 1 yr.

The model is developed for a mesoscale (10's to 100's of km) analysis. The region of study is divided into a uniform horizontal two-dimensional grid network. The rectangular grid size and number depends on the extent of the region, the desired cost/efficiency of the computer runs and the desired accuracy of analysis. Above the grids are stacked a specified number of vertical cells from the ground level to an upper limit called the mixing height. At present the model uses six vertical cells--three lower fixed-height (50 m) and three upper variable-height cells. (This arrangement is flexible and can easily be altered.) Therefore, the space enclosing the region of study is completely partitioned by a three-dimensional cell structure. The single 3D cell is the basic unit within which the model calculations are performed.

The model can handle point, line and area emission sources. The sources are assigned within one of the grids. All sources are treated simultaneously, therefore, a specific source-to-concentration/deposition value cannot be determined unless the single source is run separately. The emissions data is obtained from outside organizations (usually government control agencies). For point sources a plume rise is calculated using one of a set of five equations, and the resulting "effective stack height" is placed within the appropriate vertical cell. The meteorological condition known as lofting (effective stack height above mixing height) is accounted for. This is an important condition affecting long-range pollutant transport.

The meteorological data is obtained on tapes from the National Climatic Center (NCC) in Asheville, N.C. The tapes required are: hourly surface observations, twice daily mixing heights and hourly precipitation. This data must be consolidated and pre-processed before being useable in the model. The process is fully computerized in a set of three tape-handling programs, one for each tape, and an integrating program (METDATA) which converts the data to the hourly format required by the model.

The atmospheric boundary layer is characterized by a set of wind speed and eddy diffusivity profile equations which are calculated from ground level to the top of the mixing layer. The profiles describe the transport and diffusion behavior of the pollutants and are assumed to be vertically variable but horizontally uniform and constant across the region of study over a 1 hr period. The profiles are dependent on the stability of the atmosphere. The boundary layer has been subdivided into a surface layer and a second layer up to the mixing height. Therefore, each profile has two forms, one above and one below the surface layer. The surface layer equations are based on the Monin-Obukov (1954) similarity theory. In the upper layer the wind profile is a form of the power-law and the diffusivity is assumed constant. The profiles are calculated from a knowledge of the geostrophic wind speed, net heat flux to the ground and surface roughness. The geostrophic wind is calculated from a knowledge of the surface wind speed and height at which it is measured using a modified Regula Falsi iteration scheme. The net heat flux is calculated by first using the NCC surface observations data and the Pasquill-Turner method of stability classification to determine the stability class and then assigning a heat flux value to each class. A single surface roughness value is chosen to characterize the entire region.

The chemical conversion from SO_2 to SO_4 is assumed to be first order. At present two reaction rates are used--a day value and a night value, although hourly changes are possible if the data is available.

The dry deposition is handled by means of a deposition velocity which is calculated as a function of both terrain and meteorological conditions. The deposition velocity changes hourly, but is uniform across the region. It is determined from an aerodynamic resistance which depends on the meteorological conditions close to the ground, and a surface resistance which depends on the pollutant species and nature of the surface (snow, water, vegetation, etc.). The surface resistances are input by the user and aerodynamic resistance is internally calculated from wind profile information.

The wet deposition scheme is based primarily on a model developed by Scott (1978). It assumes all precipitation forms according to the Bergeron or cold cloud process. Ice crystals form in the upper portion of the cloud and as they sweep downward through the cloud they capture cloud droplets containing SO_4 and dissolved SO_2. The S eventually incorporated into the precipitation is assumed to be drawn in through the cloud base. A set of three equations for the wet deposition removal rate are used; one for rain or snow removal of SO_4, and one each for rain and snow removal of SO_2. Because of the nature of the wet deposition scheme, the wet removal of SO_2 and SO_4 is not calculated as part of the numerical solution of the atmospheric dispersion equation as is the dry deposition. It is calculated separately because instead of considering single cells, it considers an entire column of cells from ground level to mixing height at one time. Precipitation is assumed to occur uniformly across the region. At present there is no analysis for fractional area covered by a precipitation event, though this is one of the projected improvements to the model.

A significant feature of the model is a complete set of regional mass summations within the main program. Their purpose is first, to continually double-check to ensure mass is conserved at all stages during the internal calculations and second, to provide the basis for deriving a regional atmospheric S budget for the modeled emissions sources within the region.

There are several computer techniques worth noting. First, to handle the numerical calculations for arbitrary wind directions a feature of the model is a dual grid system, one fixed in position and one which overlaps it and rotates with the wind angle. Transfers of concentrations are performed back and forth between the two systems as the wind direction shifts. Second, the main program has a "stop-start" capability such that progress can be stopped anywhere in the stream of calculation and started exactly where it left off with no outside intervention other than re-starting the run. Third, extensive use has been made of common blocks and the "FORTRAN Procedure (PROC)" statement to eliminate unnecessary interprogram storage locating calls and to make it easier to make internal changes which affect many programs at once. Fourth, a very complete record of the values of all significant variables is stored on tape hourly for future analysis. The saved information includes the date, ground level concentration and deposition arrays, and certain meteorological, emissions and regional mass balance data. All this is compactly stored for each hour as a record of a tape file. The file covers the entire time period of simulation.

The model results include--3-hr, 24-hr, seasonal and annual average ground level concentrations, and dry, wet and total depositions of SO_2 and SO_4. (These are the standard averaging periods but the model is easily capable of also averaging upper level concentrations or using other time periods). The results also include--pH of the precipitation during a storm event, and the values and dates of the 3-hr and 24-hr maximum concentrations. All of the above results are printed grid by grid in an array format and can be isopleth computer plotted. The results also include--a frequency distribution of concentration/deposition values for any selected grid, and finally, a regional atmospheric S budget which analyzes, by total mass and percentage of S input, the flow of S (SO_2 and SO_4) through the various physical and chemical processes into, out of or within the region. This is especially useful for determining intra-region vs. extra-region impacts.

The model is written in ASCII Fortran and has been run on the Madison Academic Computing Center's SPERRY UNIVAC 1100/82 series computer. In an application of the model to the BWCA wilderness area in northern Minnesota in which a cell structure of 11 x 13 x 6 was used and in which hourly changes in meteorological data were used and in which calculations were carried out every 20 min, and in which the main program required 50K core space, a 1 yr simulation cost $200 (at the cheapest computer rate) and took

6 hr of CPU time. A 1 day calculation at the "normal" rate (10x the cheapest) can be done for $7 and takes 1 min CPU time.

For the user's reference, Table 1 contains a summary of the above discussed model features and Appendix B contains a summary of the main user-supplied input variables required to run the model.

TABLE 1. SUMMARY OF MODEL FEATURES

Feature	Description
General	- cell-type model - time-dependent (hourly) - mesoscale analysis (10's to 100's km)
	- run in batch mode
	- numerically solves coupled SO_2 and SO_4 conservation of mass equations for a dilute species in the atmospheric boundary layer described in an Eulerian frame of reference
	- includes physical processes of: wind transport turbulent diffusion chemical reactions source input dry deposition wet (rain or snow) deposition
	- uses 2D uniform horizontal grid network over region of study, uses set of 6 (3 fixed at 50 m and 3 variable) 3D cells in the vertical height from ground to mixing height
	- emission data is input once, met data is input hourly, model calculates at 20 minute intervals within an hour
	- numerical solution is first-order fully implicit type
Emissions	- can handle point, line, area sources
	- treats all emission sources simultaneously

(continued)

Table 1 (continued)

Feature	Description
	- for point sources - calculates a plume rise (using one of a set of 5 Briggs or Moses-Carsons equations) - accounts for lofting condition - SO_4 stack emissions X% of SO_2 (where X is supplied by user)
Meteorological Data	- uses data tapes from National Climatic Center (NCC) - fully computerized processing of tapes to convert data to hourly format required by model
Atmospheric Boundary Layer	- characterized by set of wind speed and turbulent eddy diffusivity profiles, assumed vertically variable but horizontally uniform and constant within region over 1 hr period - theory uses concepts of stability, geostrophic wind, surface roughness and mixing height - layer divided into 2 regions--surface layer and layer between top of surface layer and mixing height - profile equations for surface layer based on Monin-Obukov (1954) similarity theory, equations for upper region based on a form of wind speed power-law and on assumed constant diffusivity - profiles function of stability (stable, neutral, unstable); stability determined using Pasquill-Turner (1961) model - profiles function of geostrophic wind; geostrophic wind determined solely from knowledge of surface wind and the height at which it is measured using a Modified Regula Falsi iteration scheme - profiles function of surface roughness; single user-supplied roughness value assumed to be constant and uniform over region

(continued)

Table 1 (continued)

Feature	Description
	- profiles function of mixing height; hourly mixing height determined from NCC Twice Daily Mixing Height tape using linear interpolation scheme - diffusivity profile based on Mixing-Length Model
Chemical Reactions	- linear and homogeneous - uses 2 conversion rates (based on work by Husar)—2%/hr (day), 0.5%/hr (night)
Dry Deposition	- uses deposition velocity of form $V_D = \frac{1}{r_a + r_s}$, where r_a accounts for atmospheric conditions and r_s for terrain - V_D assumed uniform and constant over region
Wet Deposition	- based on model by Scott (1978) - assumes only Bergeron or cold cloud precipitation development process - assumes removal over entire vertical column from ground to mixing height at once (so calculation is separate from cell-by-cell finite difference calculations) - set of 3 wet removal equations developed: 1. SO_4 rain or snow 2. SO_2 snow 3. SO_2 rain - precipitation is assumed to occur uniformly across the region and uniformly over a 1 hr period
Computer Techniques	- written in ASCII FORTRAN - uses complex set of internal total mass summations as basis for 1. continual internal conservation of mass check 2. basis of regional total atm. sulfur budget - employs dual-grid system to handle arbitrary wind directions - employs stop-start capability - employs extensive use of COMMON'S and the FORTRAN Procedure (PROC) - stores compactly on tape complete set of hour-by-hour calculations

(continued)

Table 1 (continued)

Feature	Description			
Output Results	- Ground level concentration Dry deposition Wet deposition Total deposition	SO_2 and SO_4	3-hr 24-hr Seasonal Annual	Averages
	- Ground level concentration Dry deposition Wet deposition Total deposition	SO_2 and SO_4	Maximum 3-hr Maximum 24 hr	Dates and Values
	(All the above are printed on a grid array basis and can be isopleth computer plotted)			
	- Concentration frequency distribution for any selected grid point			
	- pH of precipitation			
	- Total atmospheric SO_2/SO_4 Budget for in-region emission sources			
Cost/Time of Application	- For 11 x 13 x 6 cells, hourly meteorological and emission input, 3 time-steps/hr, 50 K computer core, a run on SPERRY UNIVAC 1100/82 series computer,			
	One year simulation: Cost = \$200 (cheapest rate) CPU Time = 6 hr			
	One day simulation: Cost = \$7 (normal rate, 10x cheapest) CPU Time = 1 minute			

SECTION 3

OVERVIEW OF MODELING OPERATION

This section is an examination of the total modeling operation. It discusses programs, subroutines, input data and output results, the sequence of program execution, and storage modes and formats (Figure 1).

There are five major components to the modeling effort.

1. Development of emissions inventory
2. Development of meteorological data-base
3. Simulation of atmospheric transport, diffusion, chemical reactions and deposition
4. Processing of hour-by-hour concentration and deposition output
5. Isopleth computer plotting

In all there is a collection of 11 programs, 11 subroutines, and one FORTRAN PROC used. They are stored in a program file called UWATM*ACIDRAIN. Each of the above tasks are briefly discussed to give the user an overview of the entire sequence of model operation. The details are presented in the remaining sections.

EMISSIONS INVENTORY

The model is capable of handling point, line and area sources. A detailed methodology for converting agency inventories to a model useable form has been worked out only for point sources. Line and area source emissions are grid apportioned but a detailed methodology has not been included here. The emission discussions therefore directly address only point sources.

For each point source the model requires a set of six variables: location, stack height, stack diameter, gas temperature, gas flow-rate and emission rate. There are five steps involved in converting outside inventory data to the model useable form.

1. Obtain complete inventories from outside organizations
2. Select largest sources
3. Combine sources
4. Locate sources within grid network
5. Convert data to model format

Carrying out these steps involves compiling four tables and executing two programs. The first two tables are a record of what data was selected for use from the original inventories and a record of all alterations (and

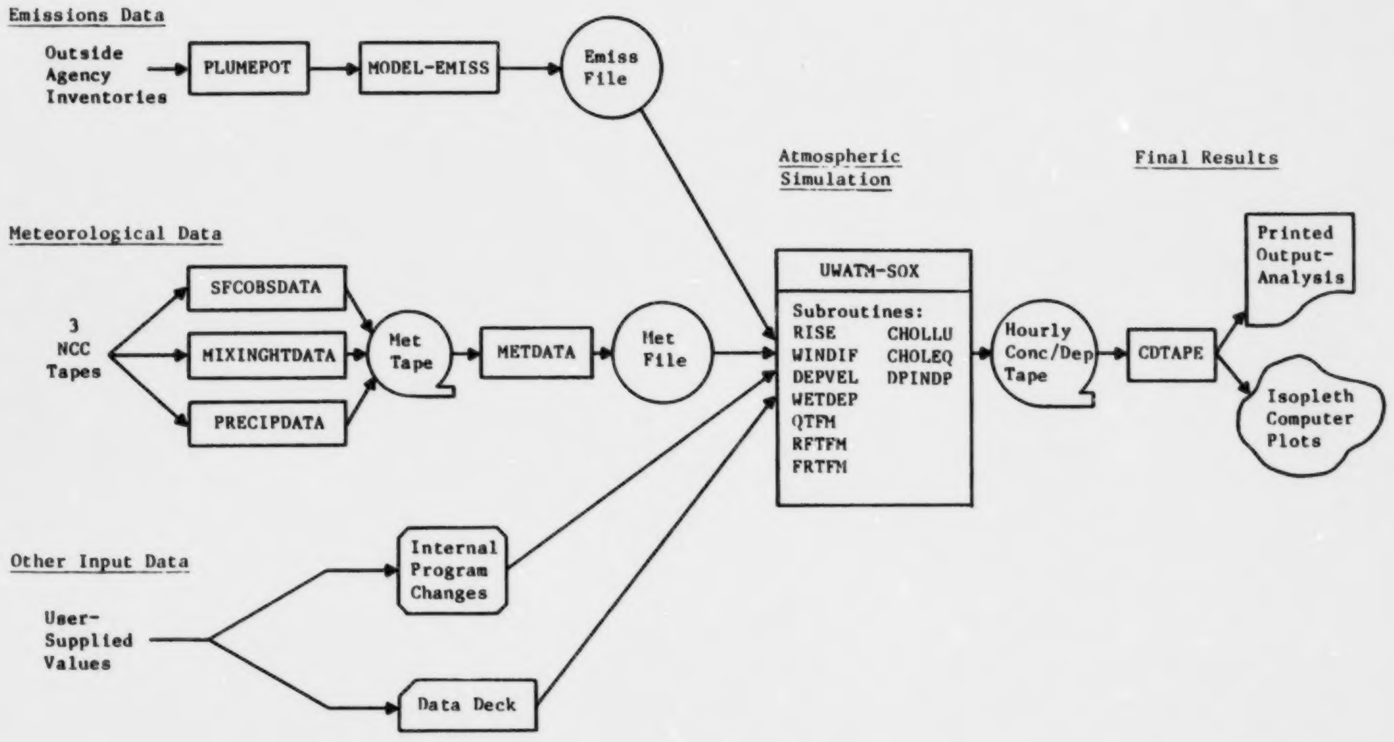
Emissions Data
Outside Agency Inventories
PLUMEPOT
MODEL-EMISS
Emiss File
Meteorological Data
3 NCC Tapes
SFCOBSDATA
MIXINGHTDATA
PRECIPDATA
Met Tape
METDATA
Met File
Other Input Data
User-Supplied Values
Internal Program Changes
Data Deck
Atmospheric Simulation
UWATM-SOX
Subroutines:
RISE
WINDIF
DEPVEL
WETDEP
QTFM
RFTFM
FRTFM
CHOLLU
CHOLEQ
DPINDP
Hourly Conc/Dep Tape
Final Results
CDTAPE
Printed Output-Analysis
Isopleth Computer Plots

Figure 1. Schematic of entire modeling operation.

reasons for) made in the process of selection. For each of the selected sources a "potential plume rise" is calculated (using a program called PLUMEPOT) and this value is used as the basis of combining sources to reduce the inventory to manageable size (if necessary). The second two tables are a record of the combined sources and a record of all alterations (and reasons for) made in the process of combining. After compiling these tables the only remaining task is to grid locate the source. This is done by hand, using U.S. Geological Survey maps. The resulting grid ID numbers are recorded on the combined sources table. Future plans call for automating this hand procedure. Finally, a program called MODEL-EMISS takes the combined sources data and changes units if necessary and places the final model emissions inventory on a mass storage file which is directly accessed by the model.

METEOROLOGICAL DATA-BASE

The model requires a set of seven hourly meteorological variables: stability, heat flux, wind speed, wind direction, air temperature, mixing height, and precipitation. All are directly or indirectly obtained from a set of three National Climatic Center (NCC) tapes. There are three steps involved in converting the original NCC tape data to the model useable form:

1. Purchase hourly surface observations, twice daily mixing height, and hourly precipitation tapes from NCC for a given meteorological station and given year
2. Pre-process data with set of three UDH programs
3. Execute METDATA program

Each of the NCC tapes are run through a separate Unified Data Handler (UDH) program (called SFCOBSDATA, MIXINGHTDATA, PRECIPDATA), which together extract the hourly wind speed, wind direction, air temperature, cloud cover, ceiling height, precipitation, and afternoon mixing height data. The data is stored as three files on another user-supplied tape which is accessed by the METDATA program. This program performs several jobs: 1. it uses the Pasquill-Turner (1961) stability class model to determine the hourly stability, 2. it uses the basic earth-sun angular equations to calculate sunrise and sunset times and solar altitude (which are used both in the stability and mixing height determination), 3. it uses a simple linear interpolation scheme to estimate hourly mixing height values, 4. it determines precipitation type (rain or snow), 5. it assigns hourly heat flux values on the basis of wind speed and stability information, 6. it converts the units of wind speed, direction and air temperature, and finally, 7. it stores all the hourly values for an entire year on a mass storage file which is directly accessed by the model.

ATMOSPHERIC TRANSPORT, DIFFUSION, CHEMICAL REACTION, AND DEPOSITION SIMULATION

This component is "the model." It consists of one main program and 10 subroutines. These contain the computer code equivalent of the mathematical equations expressing the wind transport, turbulent diffusion, chemical transformation and dry and wet deposition processes of affecting SO_2 and

SO_4. The central equation is a pair of coupled continuity equations for dilute pollutant species in the atmospheric boundary layer described in an Eulerian (or fixed) reference system. The simulation technique is a first-order fully implicit solution of the finite difference form of the coupled equations.

The differential equations used are:

$$\frac{\partial C_1}{\partial t} = -u \frac{\partial C_1}{\partial x} + K_y \frac{\partial^2 C_1}{\partial y^2} + \frac{\partial}{\partial z} (K_z \frac{\partial C_1}{\partial z}) - kC_1 + E_1 \qquad (1)$$

$$\frac{\partial C_2}{\partial t} = -u \frac{\partial C_2}{\partial x} + K_y \frac{\partial^2 C_2}{\partial y^2} + \frac{\partial}{\partial z} (K_z \frac{\partial C_2}{\partial z}) + \frac{MW_2}{MW_1} kC_1 + E_2 \qquad (2)$$

where C_1, C_2 are instantaneous concentrations of SO_2 and SO_4, respectively at a given location (x,y,z) and time t
x is downwind direction
y is crosswind direction
z is upward vertical
u is u(z) j wind speed
K_y is $K_y(z)$ is lateral turbulent momentum diffusivity
K_z is $K_z(z)$ is vertical turbulent momentum diffusivity
k is chemical reaction rate constant
MW_1, MW_2 are molecular weights of SO_2 and SO_4, respectively
E_1, E_2 are emission rates of SO_2 and SO_4, respectively at a given (x,y,z,t)

The finite difference form is explained in Section 6. For a region which has been partitioned by a 3D cell structure, the equations are solved in a downwind-step (x-step) and time-step (t-step) fashion. They are solved for one complete block of cells in the yz-plane and within the block they are solved for each t-step for the specified number of steps (currently three, thus calculating at 20-min intervals). This procedure is repeated block by block from the upwind edge to the downwind edge of the region (see Figure 5). The matrix solution for one x-step and one t-step can be symbolized as:

$$[C] = [A]^{-1}[D] \qquad (3)$$

where [C] contains the unknown concentrations,
[A] the known meteorological, chemical and deposition data and
[D] the known concentrations from the previous x-step and t-step.

This matrix equation is solved for each x-step and each t-step in the whole region for a 1 hr period, then repeated with new input data. The whole process is then repeated hour after hour until the end of the simulation period. All these calculations are performed in the main program (UWATM-SOX) with the help of three matrix handling subroutines (CHOLLU, CHOLEQ, DPINDP).

To arrive at the solution, numerous subsidiary calculations (mainly carried out by the subroutines) must be performed. These include:

1. For point sources, calculating a plume rise and determining if lofting occurs (RISE subroutine)
2. Calculating the wind and diffusivity profiles (WINDIF subroutine)
3. Calculating the deposition velocity (DEPVEL subroutine)
4. Calculating the wet deposition removal (WETDEP subroutine)
5. Shifting emission source coordinates as wind direction changes (QTFM subroutine)
6. Transfering concentrations between the dual fixed and rotating cell systems as wind direction changes (FIXROT and ROTFIX subroutines).

Each of the seven subroutines is discussed in sections 10, 7, 8, 8, 11, 11, 11, respectively.

OUTPUT PROCESSING

The main program outputs on tape hourly ground level concentration arrays, dry and wet deposition arrays, certain meteorological data, the wind and diffusivity profiles, certain emissions data and certain total regional mass calculations. A program called CDTAPE (for concentration/deposition tape processor) does all the summing, averaging and other manipulations of the hourly output. The program is complex but highly flexible. (A complete list of currently available output is given in Table 5.) Besides printing the results, CDTAPE stores them on tape in a format suitable for computer isopleth plotting.

COMPUTER PLOTTING

Our group uses the WISMAP2 computer graphics package developed by the University of Wisconsin Cartography Laboratory. To use this package it is first required that an outline map of the region of study be "digitized." Once this is done a wide variety of plotting techniques are available through WISMAP2. The plotting process will not be explained in detail because it is assumed users will have at their disposal other similar plotting packages.

SECTION 4

EMISSIONS DATA-BASE

This section explains step-by-step the methods used to select and process the emissions information needed for the model after it has been obtained from the appropriate outside organizations. Each step will be explained so it is clear what judgements are made about it and how it is altered. The starting point is emission inventories obtained from outside organizations and the end point is a "Model Emissions Inventory" containing all the emissions data needed for direct model input.

The model can handle point, line and area sources, but applications so far have called for considering only point sources. Therefore these are the only type for which a detailed methodology has been worked out. Future applications will include line and area sources. Therefore, in this section only point sources are discussed. The model requires a set of six emission variables for each point source: location coordinates (usually UTM), stack height, stack diameter, stack gas temperature, stack gas flow-rate and emissions rate. All emissions data are obtained from outside agencies. It is usually provided in the form of computer print-outs or tapes which list the needed data. No effort is made to doublecheck or verify any of the data.

There are five main steps involved in selecting and transforming the data.

1. Obtain complete emission inventories for region of study from appropriate organizations
2. Select the largest sources
3. Combine sources
4. Locate the sources in grid network
5. Convert all data to model format

Each step will be explained. Figure 2 schematically shows the methodology.

ORIGINAL INVENTORIES

The first step is to contact the appropriate agencies collecting pollutant emissions data in the region of interest. Most likely this will be federal, state or local government environmental agencies, regional planning commissions, consulting firms or special project groups. The above required variables are generally readily available. Usually hourly changes in temperature, flow-rate and emissions are not available, a single value is given for a year. Because the model is time-dependent, the rather sweeping

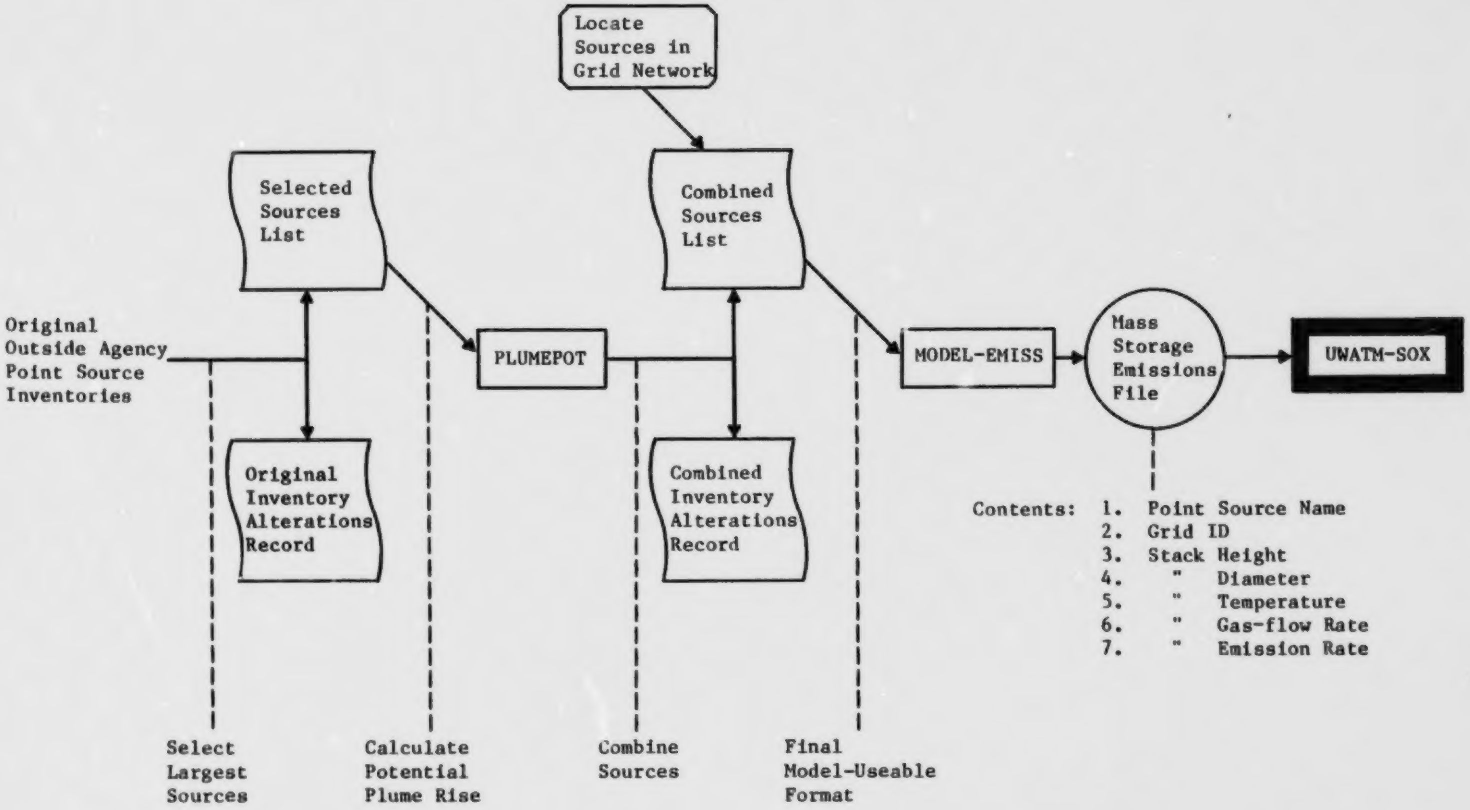
Locate
Sources in
Grid Network
Selected
Sources
List
Combined
Sources
List
Original
Outside Agency
Point Source
Inventories
PLUMEPOT
MODEL-EMISS
Mass
Storage
Emissions
File
UWATM-SOX
Original
Inventory
Alterations
Record
Combined
Inventory
Alterations
Record
Contents: 1. Point Source Name
2. Grid ID
3. Stack Height
4. " Diameter
5. " Temperature
6. " Gas-flow Rate
7. " Emission Rate
Select
Largest
Sources
Calculate
Potential
Plume Rise
Combine
Sources
Final
Model-Useable
Format

Figure 2. Schematic of emissions data methodology.

generalization must be made that they are constant over an entire year (or time period of simulation).

From the inventories for a specified pollutant, year and region the relevant variables to extract are: source ID, subunit ID (if one source has more than one emitting point), point source establishment name, UTM-coordinates, stack height, diameter, temperature, flow-rate and emissions rate.

SELECTING LARGEST SOURCES

For the sake of efficiency not all emitting points are considered separately, especially if they are numerous. It is best to establish a cut-off and consider only plants which have total emissions larger than this cut-off. If the size of the region is large (meso- or macroscale), then it is assumed the smaller sources will contribute negligibly to the longer range transport. In this case a cut-off of 100 tons/yr might be appropriate.

The point source information is selected from the original inventories and listed in a table. This table, the first actual hand-work of the emissions methodology, is called the "Selected Sources List." (See Appendix A for a sample copy suitable for xeroxing.) One plant may have more than one stack or emission generating subunit* (boiler, furnace, industrial process, etc.). Each stack or subunit is usually listed as a separate record in the agency inventories, and each should be listed separately on the Selected Sources List. Any subunit may generate less than the cut-off but if the total for the plant is greater than the cut-off all subunits are considered.

When extracting the necessary data a few alterations are made. First, for any stacks with identical characteristics the emissions are added together and only one stack is listed. Second, any stack with very small emissions (relative to the cut-off) is lumped into one of the larger stacks. A guess is made as to which larger stack seems most appropriate if there are several. Third, if a source has a measured emission value (vs. estimated or emission-factor calculated), this value is used. While making up the Selected Sources List a complete record is made of all the above small changes and any other changes, guesses, difficulties, comments which somehow relate to the alteration of the original data. This record is called the "Original Inventory Alterations Record." (See Appendix A for a sample copy suitable for xeroxing.)

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*Usually in the text the word "stack" is used instead of "subunit" whether or not it actually means a separate actual stack. Stack is a more familiar and defining term though it may not always be strictly correct.

COMBINING SOURCES

The sources in the Selected Sources List can be combined and the number thereby reduced by calculating a "potential" plume rise for each source and grouping those which have similar potentials. The equation used for this calculation is very simple.

$$\text{Rise Potential} = \frac{\text{HSTK} \cdot \text{GFLOW} \cdot \text{TS}}{\text{DIA}} \times 10^{-10} \qquad (4)$$

where HSTK is height (ft)
GFLOW is flow-rate (cfm)
TS is temperature (deg R)
DIA is diameter (ft)
10^{-10} is a factor to reduce the resulting large number to about 1; is not a units conversion

The equation is linear in every term. It is not an experimentally derived equation, though it roughly accords with the typical plume rise equations in common use. It is used purely as a simple aid to combining sources. A computer program called PLUMEPOT executes the equation for every source. Sections 12 and 13 discuss how to run the program.

The actual combining is done by hand. The decision to combine is subjective and involves comparing the plume rise potentials, the emissions, the location and any other relevant information. Generally, similar potentials (± 50%) for stacks within one plant are grouped together. Subunits with small emissions may be combined with larger. Sources within the same area may be grouped. When combining, either the stack characteristics of the largest emitter or an average of all combined emitters can be used, whichever is deemed most appropriate. Out of these judgements emerges a reduced list of sources recorded in a new table called the "Combined Sources Inventory." While making up this list a complete record is made of what is combined and why. This record is called the "Combined Inventory Alterations Record." (See Appendix A for sample copies of each data sheet suitable for xeroxing.)

LOCATING THE SOURCES

The source location is known by UTM (Universal Transverse Meridian) coordinates. These coordinates are used because they refer to a rectangular grid system, and it is easier for modeling purposes to visualize in terms of grids than in longitude and latitude (where the spacing varies with location). Also, the UTM coordinates are more accurate for smaller scales than longitude and latitude. The model requires that the sources be located within one of the model grids which subdivide the region.

The process of assigning a source to a particular grid is currently done by hand. It is simple once one learns how to read UTM-coordinates on a U.S. Geological Survey (USGS) map. The grid system is drawn on a transparency which is placed over the USGS maps which cover the region. The sources are then located on the map and the ID of the grid within which the source lies is recorded on the Combined Sources Inventory under the heading "Grid Coordinates." Section 12 explains the method of grid ID assignment.

The method of locating the sources is presently done by hand but our plan is to develop a computer program which can automatically find the correct grid ID. All that is basically needed for this is the UTM-coordinates of the corners of the grid system and the grid size. When only a small number of sources are involved the hand method is adequate.

FINAL MODEL FORMAT

The Combined Sources Inventory data sheets contain all the information needed by the model, except the units are usually not correct. (The original units are usually English and the model uses metric.) The data sheets are prepared for computer use, as explained in Section 12, for input to a program called MODEL-EMISS. This is the final step in the emissions inventory process. The program converts the units to the required metric units and stores the values in the proper format as an element of a mass storage file. Sections 12 and 13 discuss how to run the program.

SUMMARY

The final product of the emissions data processing is a mass storage file which contains for every combined point source in the region the following information.

1. Point source name
2. Grid ID
3. Stack height (m)
4. Stack diameter (m)
5. Stack gas temperature (°K)
6. Stack gas flow-rate (m^3/sec)
7. Emissions rate (g/sec)

Note that the end results not only include the model inventory but also a complete record of all alterations to the original data made by the user. This is contained on the Original Inventory Alterations Record and Combined Inventory Alterations Record. These may prove useful to the user when the time comes to compare model results to monitoring data. It will remind the user of accuracy limitations in the emissions data that may have affected the model results. Figure 2 illustrates schematically the emissions methodology.

SECTION 5

METEOROLOGICAL DATA BASE

This section explains where to obtain the meteorological data and the methods used to select and process it for model use. Each step is explained so it is clear how the data is transformed from the original NCC tapes to the final hourly data-base needed for direct model input.

The model requires a set of seven hourly meteorological variables: wind speed, wind direction, stability, heat flux, air temperature, mixing height and precipitation. All seven may be obtained directly or indirectly from a set of three NCC tapes. This data must pass through two sets of programs, first, a set of three Unified Data Handler (UDH) programs (one for each tape) and second, a program called METDATA which does the necessary calculations and stores the data in the proper format for the model.

There are three major steps involved in obtaining and processing the data.

1. Purchase NCC tapes
2. Run UDH programs
3. Run METDATA program

Each step will be explained. Figure 3 schematically shows the methodology.

NCC TAPES

From the NCC the following three types of magnetic tapes are ordered.

1. Hourly surface observations*
   Tape is called: TD-1440
   Airways Surface Observations
   Card Image 144, Block 10
   Cost is approximately $85

---

*A special comment must be about the surface observation tape. Generally it is available only for 3-hr observations instead of hourly, but some stations have hourly processed data. Be sure to ask if the 24 observations/day vs. 8 observations/day is available.

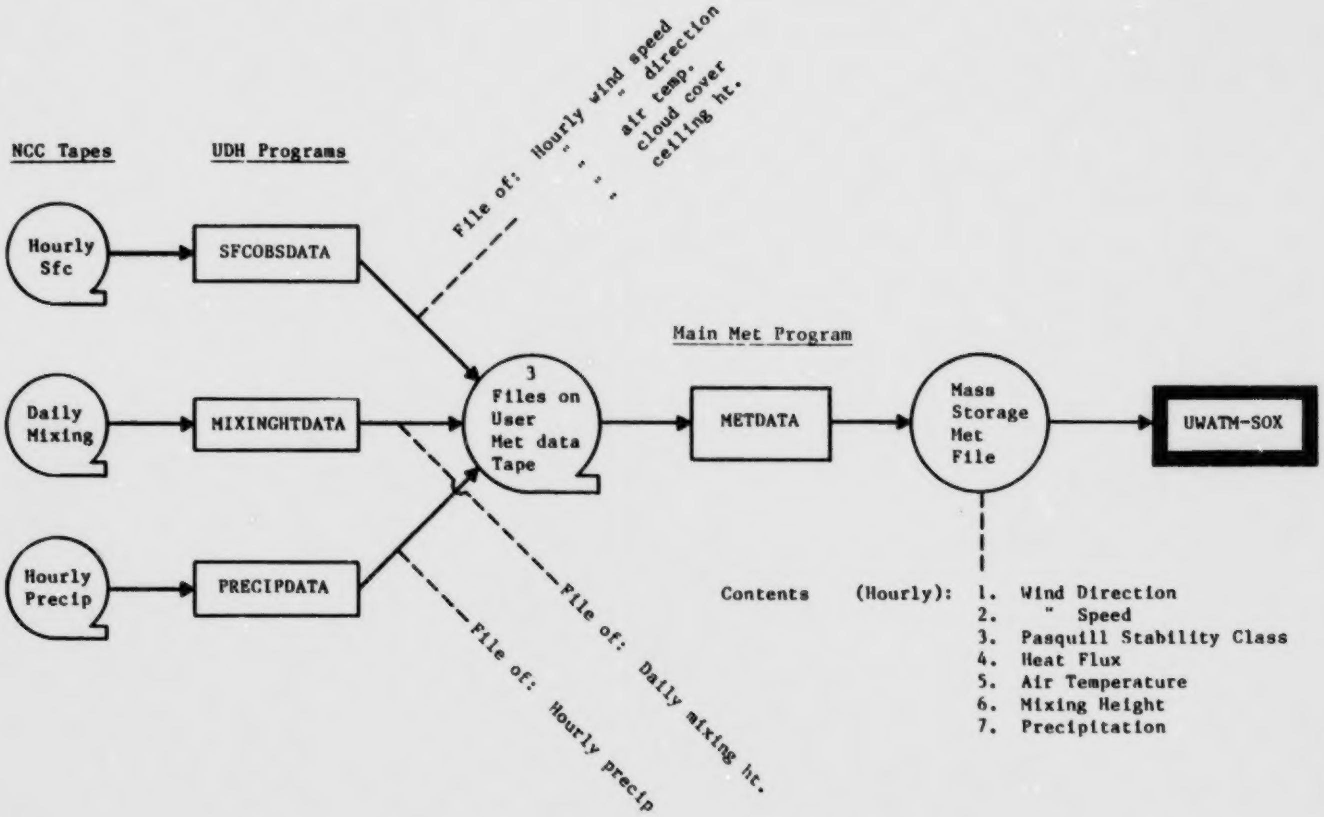

NCC Tapes
UDH Programs
Hourly Sfc
Daily Mixing
Hourly Precip
SFCOBSDATA
MIXINGHTDATA
PRECIPDATA
File of: Hourly wind speed
" " direction
" " air temp.
cloud cover
ceiling ht.
File of: Daily mixing ht.
File of: Hourly precip
3 Files on User Met data Tape
Main Met Program
METDATA
Mass Storage Met File
UWATM-SOX
Contents (Hourly): 1. Wind Direction
2. " Speed
3. Pasquill Stability Class
4. Heat Flux
5. Air Temperature
6. Mixing Height
7. Precipitation

Figure 3. Schematic of meteological data methodology.

2. Twice daily mixing heights
   Tape is called: TD-9689
   Daily Mixing Heights
   Cost is approximately $85

3. Hourly precipitation
   Tape is called: TD-9657
   Hourly Precipitation
   Card Image 488
   Cost is approximately $85

Order all tapes 9-track, 1600 BPI, EDCDIC.

The address to send to is: National Climatic Center
Federal Building
Asheville, N.C. 28801
(704) 258-2850

For each tape the stations and years desired must be specified. A list of all stations and years is available from NCC.

UDH PROGRAMS

Madison Academic Computing Center (1979) provides a software system designed to manipulate data in a simple and efficient manner. It can carry out a wide range of operations such as transfering data between external media; sorting, selecting, merging, summarizing, updating data; manipulating individual items of data including substitution of values and arithmetic computations; and prepare input data for other software systems. It was developed at the University of Wisconsin-Madison. This software system was chosen as most appropriate for the simple processing operations required here.

The three programs are called SFCOBSDATA, MIXINGHTDATA and PRECIPDATA and each processes one of the three tapes and stores the processed information as a file on a user-supplied tape. The met data from the NCC tapes is handled similarly by each of the UDH programs. The five main functions performed in these programs are as follows:

1. Selecting off the tapes the relevant variables, dropping unneccessary ones
2. Double checking that year and met station ID's are correct
3. Making changes in certain character notations
4. Formating data in appropriate form for the METDATA program
5. Outputing the data onto the user's tape

The logic of the programs is simple and straightforward and is not discussed. Sections 12 and 13 describe how to run the programs.

METDATA PROGRAM

This program uses the three UDH-created tape files to create the hourly meteorological data-base needed by the model. From the original NCC data the UDH programs select and process the following variables: year, month, day, hour; hourly values of wind speed, wind direction, air temperature, cloud cover, ceiling height and precipitation; and daily values of afternoon mixing height. METDATA uses these as input, and outputs the following seven variables: Pasquill stability class number, mixing height, precipitation, air temperature, heat flux, wind speed and wind direction.

There are five tasks which the METDATA program performs:

1. Stability class determination
2. Mixing height interpolation
3. Precipitation typing
4. Heat flux assignment
5. Wind speed, wind direction and air temperature units conversion.

Each of these is discussed individually.

Stability Class Determination

Stability is a measure of the level of turbulence. A method of determining stability from common ground level observations was devised by Pasquill (1961) and modified by Turner (1964). According to this method there are seven stability classes. To determine the class two main variables must be known--net radiation to the ground and wind speed. The net radiation is dependent on four subsidiary variables: if it's day or night, solar altitude, cloud cover and ceiling height. The following procedure with accompanying tables is used by the program and is known as the Pasquill-Turner Stability Class Method. This procedure requires the Net Radiation Index be determined by:

A. If the total cloud cover is 10/10 and the ceiling is < 7000 ft use net radiation index equal to 0 (whether day or night).
B. For night-time (night is defined as the period from 1 hr before sunset to 1 hr after sunrise):
    1. If total cloud cover $\leq$ 4/10, use net radiation index equal to -2.
    2. If total cloud cover $>$ 4/10, use net radiation index equal to -1.
C. For daytime:
    1. determine the insolation class number as a function of solar altitude from Table 2.
    2. If total cloud cover $\leq$ 5/10, use the net radiation index in Table 3 corresponding to the insolation class number.
    3. If cloud cover > 5/10, modify the insolation class number by following these six steps:
        a. Ceiling < 7000 ft subtract 2.
        b. Ceiling $\geq$ 7000 ft but < 16,000 ft subtract 1.
        c. Total cloud cover equal 10/10, subtract 1. (This will only apply to ceilings $\geq$ 7000 ft since cases with 10/10 coverage below 7000 ft are considered in item 1 above.)

d. If insolation class number has not been modified by steps 1., 2., or 3. above, assume modified class number equal to insolation class number.
e. If modified insolation class number is < 1, let it equal 1.
f. Use the net radiation index in Table 3 corresponding to the modified insolation class number.

TABLE 2. INSOLATION AS A FUNCTION OF SOLAR ALTITUDE

Solar altitude (a)	Insolation	Insolation class no.
$60° < a$	Strong	4
$35° < a \leq 60°$	Moderate	3
$15° < a \leq 35°$	Slight	2
$a \leq 15°$	Weak	1

TABLE 3. STABILITY CLASS AS A FUNCTION OF NRI VS. WIND SPEED

	Net radiation index[a]						
Wind speed (knots)	4	3	2	1	0	-1	-2
0, 1	1	1	2	3	4	6	7
2, 3	1	2	2	3	4	6	7
4, 5	1	2	3	4	4	5	6
6	2	2	3	4	4	5	6
7	2	2	3	4	4	4	5
8, 9	2	3	3	4	4	4	5
10	3	3	4	4	4	4	5
11	3	3	4	4	4	4	4
$\geq$ 12	3	4	4	4	4	4	4

[a] Radiation indices are 1. extremely unstable, 2. unstable, 3. slightly unstable, 4. neutral, 5. slightly stable, 6. stable, 7. extremely stable.

Therefore, given hourly data for wind speed, cloud cover, ceiling height, and solar altitude, and if the hour is day or night, hourly values can be determined for the stability class number using the above procedure. The first three variables are furnished directly from the hourly surface observations tape, but the last two must be calculated.

The calculations needed are: 1. sunrise and sunset times (to compare to the given hour to determine if it's day or night) and 2. if daytime, the solar altitude. Both are determined using the same set of equations describing the angular relation between the earth and sun. The following is the basic Earth-Sun Angular Relationship (Duffie and Beckman 1980) equation:

$$\cos \theta_z = \sin \delta \sin \phi + \cos \delta \cos \phi \cos \omega \quad (5)$$

where θ_z is zenith angle (angle between a beam from the sun and the straight overhead vertical--thus the angle is always positive and between 0° and 90°)

δ is declination (angle between the sun at solar noon--solar noon is the highest position of the sun during the day and does not necessarily and most often would not correspond to 1200 hours and the plane of the equator) (north is positive) and is $23.45 \sin \left(360 \times \frac{284 + n}{365}\right)$; where n is day number of the year (1 through 365 or 366) δ is declination in degrees

ϕ is latitude (positive in northern hemisphere)

ω is hour angle (angle between position of sun at solar noon and some other specified time--solar noon is 0°, each hour is 15° of longitude with morning defined negative and afternoon positive, e.g., $\omega = -15°$ for 1100 hours, $\omega = +37.5°$ for 1430 hours)

Note that the values for the zenith angle, which primarily determines incident radiation on the earth, changes with time of day (hour angle), with the time of year (declination angle), and with location (latitude). This equation can be manipulated to yield the desired equations for sunrise and sunset times and solar altitude.

All the equations and data necessary to determine the hourly stability class according to the Pasquill-Turner model is now available. To summarize, the two main variables needed are net radiation and wind speed. Wind speed is known from the data tape. To indirectly estimate net radiation, the cloud cover, ceiling height, solar altitude and whether it is day or night must be known. Cloud cover and ceiling height are known from the data tape. Day night is found by comparing the given hour to the sunrise and sunset times. To find these times the earth-sun angular equations are used and the day number, latitude and longitude of the point of interest and the standard meridian for the local time zone must be known. These are easily found or calculated. To know the solar altitude requires no additional information beyond that needed for the day night calculations. The solar altitude finally is used in conjunction with the cloud cover and ceiling height to give a net radiation index which is in turn used with wind speed to determine the stability from Table 3 above. In conclusion, the only user input-data required for the Pasquill-Turner "cookbook" method are: day, hour, wind speed, cloud cover, ceiling height, latitude, longitude and standard meridian. The first five are available in the NCC Surface Observations tape, the last three are input separately.

Mixing Height Interpolation

Mixing height values are available twice daily (morning and afternoon) from the NCC data tape. They have been calculated from a measurement of the temperature profile in the first few thousand meters of the earth's surface. The problem for the modeling effort is to estimate hourly values for the mixing height from this data. This is done with a simple linear interpolation using only the afternoon mixing height value. To calculate the hourly values we need to know the following.

1. Afternoon mixing height (at 1400 hours)
2. Local standard time of sunrise and sunset
3. Hourly estimates of stability

The first is available from the NCC tape and the other two have been internally calculated in the METDATA program as part of the stability class determination. This particular interpolation method is an imitation of that used in the U.S. EPA CRSTER model for rural hourly mixing heights (U.S. Environmental Protection Agency 1977). The scheme is illustrated in Figure 4.

There are three time periods to interpolate between, and for one period two different equations are possible. The three time periods covering a whole day are: sunset to sunrise, sunrise to 1400, and 1400 to sunset. The time period with two cases is sunrise to 1400. The equation used depends on the stability 1 hr before sunrise. If neutral, the mixing height changes according to case #2 on the figure, if stable then according to case #3. Therefore, we have four possible calculations.

1. Sunset to sunrise
2. Sunrise to 1400 hours (neutral)
3. Sunrise to 1400 hours (stable)
4. 1400 hours to sunset

The interpolation equations for each case are not given.

Precipitation Type

The NCC Hourly Precipitation tape does not give the form of precipitation, only the water equivalent inches. It is necessary for the model's wet deposition scheme to know whether the precipitation is rain or snow.

Determining the type is accomplished by assuming all precipitation in a given period in either rain or snow. For instance, in a model application in northern Minnesota all precipitation in November, December, January, February, and March was assumed to be snow and the rest rain. Section 12 describes how to change the METDATA program to conform to the user's chosen precipitation-type dividing line.

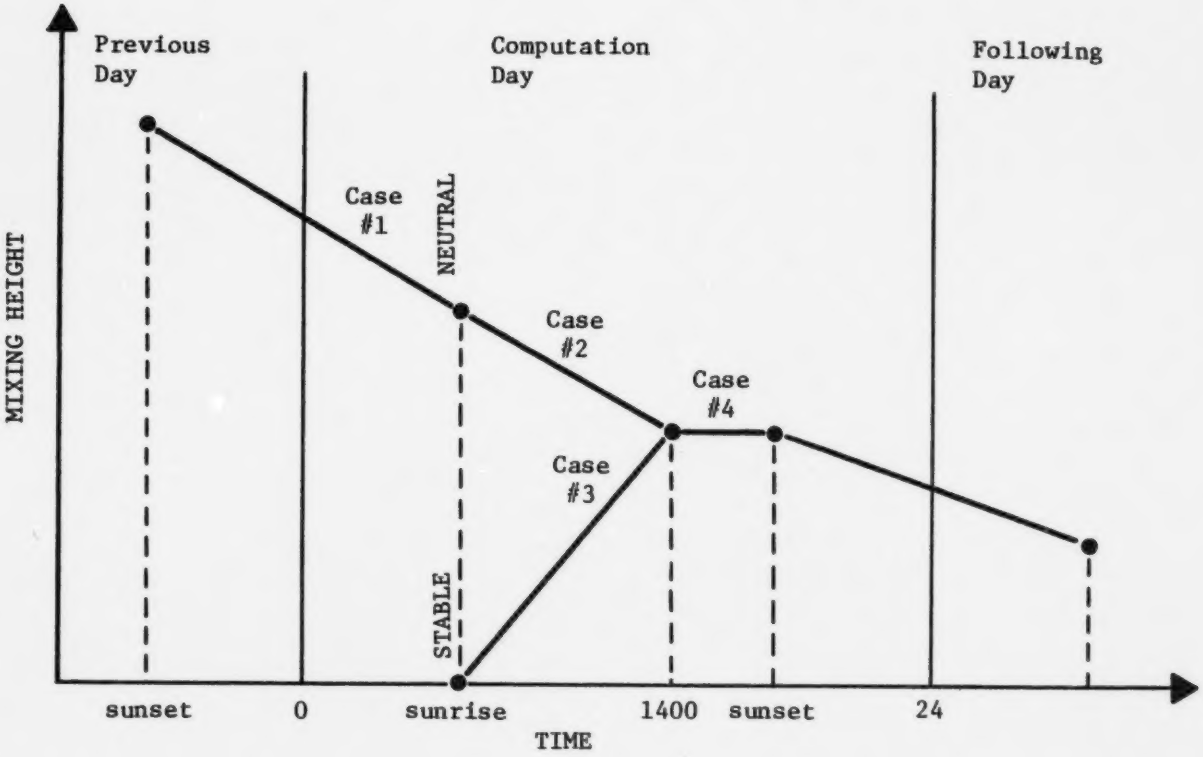

MIXING HEIGHT
Previous Day
Computation Day
Following Day
Case #1
NEUTRAL
Case #2
Case #4
Case #3
STABLE
sunset
0
sunrise
1400
sunset
24
TIME

Figure 4. Mixing weight interpolation method.

Heat Flux Assignment

The hourly values of the net heat flux to the earth's surface are assigned according to the net radiation index for the given hour as calculated in the stability section of the program. The values assigned are listed in Table 4.

TABLE 4. NET HEAT FLUX TO EARTH'S SURFACE

NRI	Heat flux (cal/cm^2/sec)
4	0.24
3	0.18
2	0.12
1	0.06
0	0.00
-1	-0.03
-2	-0.06

Wind Speed, Wind Direction, Air Temperature Units Conversion

The following are the conversions:

1. Wind speed is changed from knots to m/sec and then multiplied by 10 so the value to the tenth of a m/sec can be stored as an integer.

2. Wind direction is changed from tens of degrees to degrees and stored as an integer.

3. Air temperature is changed from °F to whole °K and stored as an integer.

SUMMARY

The final product of the meteorological data processing is a mass storage file which contains for every hour of a year the following information.

1. Wind direction (degrees clockwise from north)
2. Wind speed (m/sec)
3. Pasquill stability class number (1-7)
4. Heat flux (cal/cm^2/sec)
5. Air temperature (°K)
6. Mixing height (m)
7. Precipitation (1/100 in. water equivalent)

Figure 3 illustrates schematically the meteorological data-processing.

SECTION 6

ATMOSPHERIC DISPERSION -- EQUATIONS AND SIMULATION

THE DIFFERENTIAL EQUATIONS

The following are the coupled SO_2 and SO_4 conservation of mass equations for dilute pollutant species in the atmospheric boundary layer described in an Eulerian frame of reference which are used by the model.

$$\frac{\partial C_1}{\partial t} = -u \frac{\partial C_1}{\partial x} + K_y \frac{\partial^2 C_1}{\partial y^2} + \frac{\partial}{\partial z} \left(K_z \frac{\partial C_1}{\partial z}\right) - kC_1 + E_1 \qquad (6)$$

$$\frac{\partial C_2}{\partial t} = -u \frac{\partial C_2}{\partial x} + K_y \frac{\partial^2 C_2}{\partial y^2} + \frac{\partial}{\partial z} \left(K_z \frac{\partial C_2}{\partial z}\right) + \frac{MW_2}{MW_1} kC_1 + E_2 \qquad (7)$$

where C_1, C_2 are instantaneous concentrations of SO_2 and SO_4, respectively at a given point in space (x,y,z) and given instant of time t

x is downwind direction

y is crosswind direction

z is upward vertical

u is u(z) is wind speed

K_y is $K_y(z)$ is lateral turbulent momentum diffusivity

K_z is $K_z(z)$ is vertical turbulent momentum diffusivity

k is chemical reaction rate constant

MW_1, MW_2 are molecular weight of SO_2 and ionic weight of SO_4, respectively

E_1, E_2 are emission rates of SO_2 and SO_4 at a given (x,y,z,t).

These equations will be referred to as the SO_2/SO_4 Model Differential Equations. The following processes affecting pollutant behavior are represented: 1. wind transport, 2. turbulent diffusion, 3. chemical reactions, and 4. emissions input. (Note--dry deposition is implicit in the above equations as a boundary condition and wet deposition is handled separately from the above formulation.)

Some of the assumptions implicit in the equations include the following.

1. The air (N_2, O_2, CO_2, etc.) and the pollutants (SO_2, SO_4) can be described as a fluid, in other words, are assumed to form a continuum. In practice this means the infinitesimal volume element to which the equations are applied is of a size larger than the mean free path of the air particles (so the atomic discontinuities disappear) but smaller than the distance over which the atmospheric properties change significantly (so the properties can be assumed uniform within).

2. The pollutants are dilute, therefore do not affect the overall behavior of the air. This allows the continuity equations to be solved independently of the coupled momentum and energy equations.

3. Molecular diffusion is assumed negligible compared to the other processes.

4. The wind vector and concentration are inherently random variables. Therefore, u represents a time-averaged wind speed and C represents a theoretical ensemble average (Seinfeld 1975).

5. The turbulent nature is described by the Mixing Length Model, in which, in analogy to the atomic mean free path a mixing length is postulated which is the average distance over which a turbulent eddy maintains itself. The pollutant flux carried by the eddy is assumed proportional to the mean concentration gradient and the "constant" of proportionality is called the turbulent eddy diffusivity.

6. The turbulent eddy diffusivity is assumed equivalent to the turbulent momentum diffusivity which is a much easier variable to measure experimentally.

7. The atmosphere is assumed to be incompressible.

8. The chemical reactions are assumed to be first-order, homogeneous and independent of the air temperature.

9. The wind velocity is constant from one direction (x-direction) over a given time interval.

10. The wind transport in the x-direction dominates the turbulent diffusion in that direction.

11. The values of u, K_y, K_z vary only in the vertical and are constant and uniform in the horizontal plane over a 1 hr period.

THE FINITE DIFFERENCE EQUATIONS

Ideally, it would be desireable to solve the above equations for every point in space and for all time. But because of the complex form of u, K_y,

K_z they cannot be solved analytically. Therefore, a finite difference or numerical solution is dictated.

In finite difference analysis the unit of analysis is no longer the infinitesimal volume element but a volume element with finite dimensions. In modeling applications to the atmosphere dimensions can range from meters to thousands of meters. The validity of use of dimensions of this scale depends on how well the atmospheric conditions approximate the above assumptions within the finite volume of air.

The task now is to re-formulate the SO_2/SO_4 Model Differential Equations in a way which will permit simultaneous solution for concentrations in a multiple finite volume element (or multi-cell) system. Figure 5 will aid in visualizing the finite difference form. The i, j, k notation in the figure corresponds to the x, y, z directions, respectively, and represents the cell number being referred to. If the multi-cell system contains NUMX, NUMY, NUMZ cells in the three directions then i will have values of 1 to NUMX, j of 1 to NUMY, k of 1 to NUMZ. The cells dimensions are Δx, Δy, Δz. The finite difference form of each of the terms in the SO_2/SO_4 Model Differential Equations is written out below.

Wind Transport: $u_k \, (C^{t+1}_{i+1,j,k} - C^{t+1}_{i,j,k}) \, \Delta y \Delta z$

Lateral Diffusion: $K_{y_k} \left(2C^{t+1}_{i+1,j,k} - (C^{t+1}_{i+1,j+1,k} - C^{t+1}_{i+1,j-1,k}\right) \dfrac{\Delta x \Delta z}{\Delta y}$

Vertical Diffusion:

$$\left[K_{z_{k+1/2}}\left(C^{t+1}_{i+1,j,k+1} - C^{t+1}_{i+1,j,k}\right) - \right.$$

$$\left. K_{z_{k-1/2}}\left(C^{t+1}_{i+1,j,k} - C^{t+1}_{i+1,j,k-1}\right)\right] \frac{\Delta x \Delta y}{\Delta z}$$

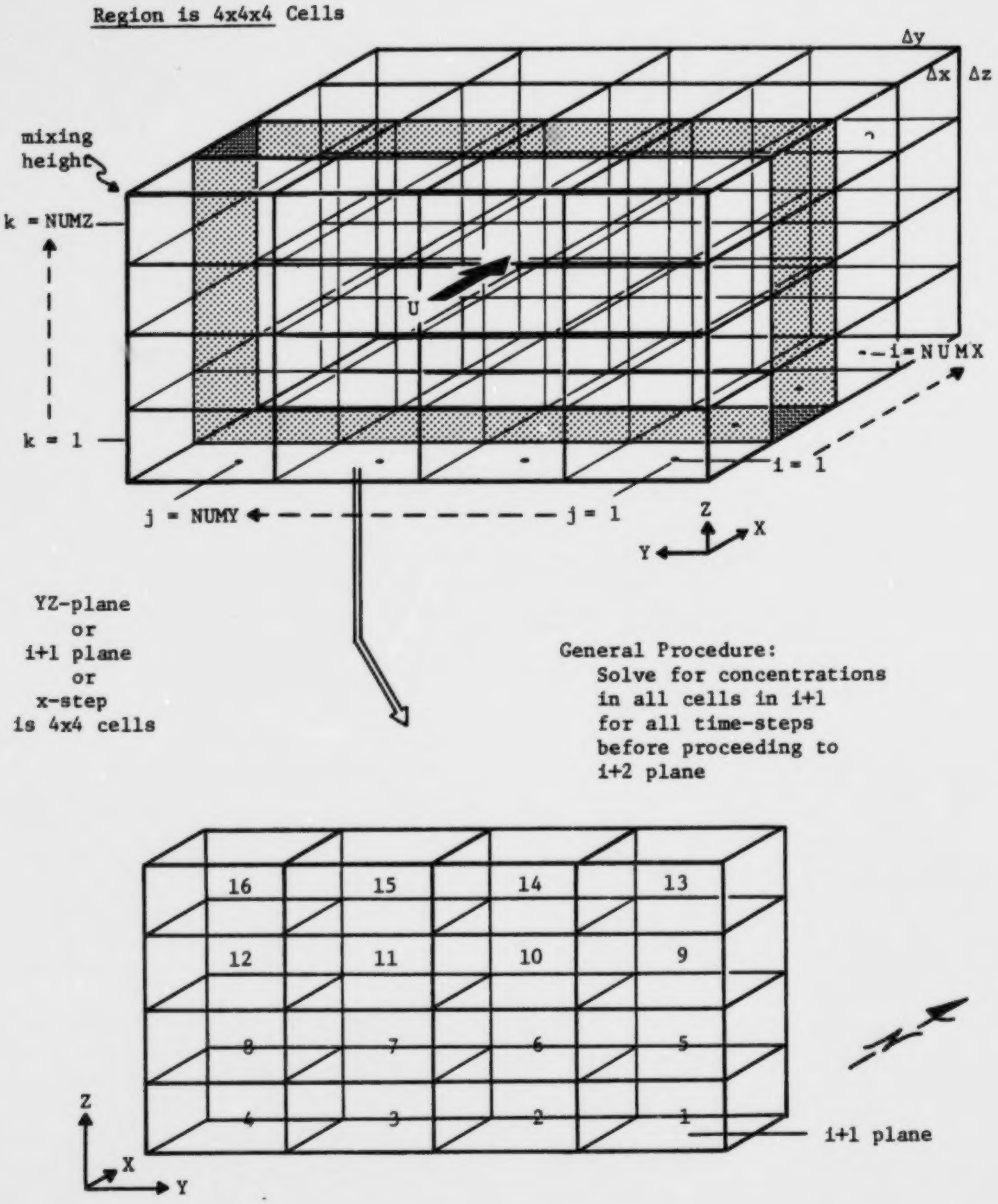
Chemical Reactions: $-K \; {}^{1}C^{t+1}_{i+1,j,k} \, \Delta x \Delta y \Delta z$ for SO_2 equation

$\dfrac{MW_2}{MW_1} K \; {}^{1}C^{t+1}_{i+1,j,k} \, \Delta x \Delta y \Delta z$ for SO_4 equation

(K is the chemical reaction rate constant, and should not be confused with K representing the diffusivities)

Sources: $Q^{t+1}_{i+1,j,k}$

Time Change: $\left(C^{t+1}_{i+1,j,k} - C^{t}_{i+1,j,k}\right) \dfrac{\Delta x \Delta y \Delta z}{\Delta t}$


Region is 4x4x4 Cells

Δy
Δx
Δz
mixing height
k = NUMZ
k = 1
U
i = NUMX
i = 1
j = NUMY
j = 1
Z
X
Y
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
i+1 plane
Z
X
Y

YZ-plane
or
i+1 plane
or
x-step
is 4x4 cells

General Procedure:
Solve for concentrations
in all cells in i+1
for all time-steps
before proceeding to
i+2 plane

Figure 5. Regional cell structure.

(Note--k represents the values of u and K_y at the center of the cell, and $k \pm 1/2$ represents the values of K_z at the top and bottom of the cell.)

Each one of these terms represents the net rate of mass change in the cell of dimensions $\Delta x \Delta y \Delta z$ due to the particular process over the time period Δt. The collection of these equations represents the total rate of mass change for either SO_2 or SO_4 for a single cell (i+1,j,k) for the time period between t and t+1.

The scheme of this model is to solve for all concentrations of SO_2 and SO_4 for all cells in the i+1 plane simultaneously for time t+1. This assumes that the concentrations for the previous i^{th} plane and for the previous t^{th} time-step (in the i+1 plane) are already known. The calculation therefore involves the simultaneous solution of equations for NUMY*NUMZ cells. This calculation is first done for all time-steps within a 1 hr period (e.g., three t-steps per simulated hour) before moving on to the i+2 plane. The t-steps are repeated again before moving on to the i+3 plane. In this downwind step-wise fashion the concentrations are calculated for every cell in the region for every time-step within 1 hr. Then the model inputs new meteorological data and the entire sequence is repeated.

This type of scheme, known as a fully implicit first-order finite difference technique, requires that the model equations be written out for each cell in a given plane. If there are 4x4 cells then 16 simultaneous equations must be solved. Of the above terms only $C^{t+1}_{i,j,k}$ (concentrations in already solved i-plane) and $C^{t}_{i+1,j,k}$ (concentrations in already solved t-step) are assumed to be known. The rest are unknown. Of course, it is assumed that from outside sources the variables u_k, K_{y_k}, K_{z_k}, K, MW_1, MW_2 and Q are known and that $\Delta x, \Delta y, \Delta z, \Delta t$ are user selected appropriate to the planned application. The entire finite difference form of the SO_2/SO_4 Model Differential Equations can now be written out.

Let 1 be SO_2
2 be SO_4
a be $u \, \Delta y \Delta z$
e be $K_y \dfrac{\Delta x \Delta z}{\Delta y}$
f be $K_z \dfrac{\Delta x \Delta y}{\Delta z}$
t be $\dfrac{\Delta x \Delta y \Delta z}{\Delta t}$
r_1 be $K \Delta x \Delta y \Delta z$
$r_2 = \dfrac{MW_2}{MW_1} r_1$

Then for SO_2,

$$(a_k + t + r_1)\,{}^1C^{t+1}_{i+1,j,k} + e_k\,\left(2\,{}^1C^{t+1}_{i+1,j,k} - {}^1C^{t+1}_{i+1,j+1,k} - {}^1C^{t+1}_{i+1,j-1,k}\right) +$$

$$f_{k+1/2}\left({}^1C^{t+1}_{i+1,j,k+1} - {}^1C^{t+1}_{i+1,j,k}\right) + f_{k-1/2}\left({}^1C^{t+1}_{i+1,j,k-1} - {}^1C^{t+1}_{i+1,j,k}\right) =$$

$$a_k\,{}^1C^{t+1}_{i,j,k} + t\,{}^1C^{t}_{i+1,j,k} + {}^1Q^{t+1}_{i+1,j,k} \qquad (8)$$

and for SO_4,

$$(a_k + t)\,{}^2C^{t+1}_{i+1,j,k} + e_k\,\left(2\,{}^2C^{t+1}_{i+1,j,k} - {}^2C^{t+1}_{i+1,j+1,k} - {}^2C^{t+1}_{i+1,j-1,k}\right) +$$

$$f_{k+1/2}\left({}^2C^{t+1}_{i+1,j,k+1} - {}^2C^{t+1}_{i+1,j,k}\right) + f_{k-1/2}\left({}^2C^{t+1}_{i+1,j,k-1} - {}^2C^{t+1}_{i+1,j,k}\right) =$$

$$a_k\,{}^2C^{t+1}_{i,j,k} + t\,{}^2C^{t}_{i+1,j,k} + {}^2Q^{t+1}_{i+1,j,k} + r_2\,{}^1C^{t+1}_{i+1,j,k} \qquad (9)$$

These equations will be referred to as the SO_2/SO_4 Model Finite Difference Equations.

INITITAL AND BOUNDARY CONDITIONS

For a complete solution of the above set of equations within a region, initial conditions and boundary conditions need to be specified. A complete listing of them is given in Table 5. They are given in both differential and finite difference form.

The model first assumes that at the initial starting time all concentrations are zero. If it is known they can be set to a uniform background value. The concentrations outside the network are at all times assumed to be zero. Again, a uniform background can also be assumed. It is assumed there is no lateral diffusion out of the sides of the region or out of the top (i.e., across the mixing height). The pollutants are perfectly reflected and hence stay within the confines of the region except when blown out of the downwind edge of the region. At ground level, pollutants are dry deposited. The flux is calculated using the deposition velocity concept explained further in Section 8.

SIMULTANEOUS EQUATIONS

The complete formulation of the simultaneous finite difference equations together with boundary conditions can be represented by the following matrix form:

$$[A_{mn}][C_n] = [D_m] \qquad (10)$$

TABLE 5. MODEL INITIAL AND BOUNDARY CONDITIONS

Process	Differential form		Finite difference form
Initial time	at $t=0$,	$C=0$	at $t=0$, $C^{o}_{i+1,j,k} = 0$
Background concentration	at $x=0$,	$C=0$	at $i=0$, $C^{t+1}_{ijk} = 0$
Lateral diffusion at edges	at $y=0$ and $y=y_{max}$	$K_y \frac{\partial C}{\partial y} = 0$	at $j=0$, $C_k\left(C^{t+1}_{i+1,j,k} - C^{t+1}_{i+1,j-1,k}\right) = 0$ and $j=\mathrm{NUMY}$, $C_k\left(C^{t+1}_{i,j+1,k} - C^{t+1}_{i+1,j,k}\right) = 0$
Vertical diffusion at mixing height	at $Z=Z_m$,	$K_z \frac{\partial C}{\partial z} = 0$	at $k=\mathrm{NUMZ}$, $f_{k+1/2}\left(C^{t+1}_{i+1,j,k} - C^{t+1}_{i+1,j,k+1}\right) = 0$
Dry deposition	at $Z=0$,	$K_z \frac{\partial C}{\partial z} = V_D C$ (where V_D = deposition velocity)	at $k=1$, $f_{k-1/2}\left(C^{t+1}_{i+1,j,k} - C^{t+1}_{i+1,j,k-1}\right) =$ $d\, C^{t+1}_{i+1,j,1}$ (where $d = V_D \Delta x \Delta y$)

The A-matrix contains the known meteorological, deposition and chemical reaction parameters. The C-matrix contains the unknown concentrations to be solved for. The D-matrix contains the known terms from the previous x-step and t-step, and the emission rates. The m and n subscripts indicate the standard row and column form of matrix expression. Therefore, since A and D contain all known terms the concentrations in the i+1-plane can be solved for:

$$[C_n] = \frac{[D_m]}{[A_{mn}]} \,. \tag{11}$$

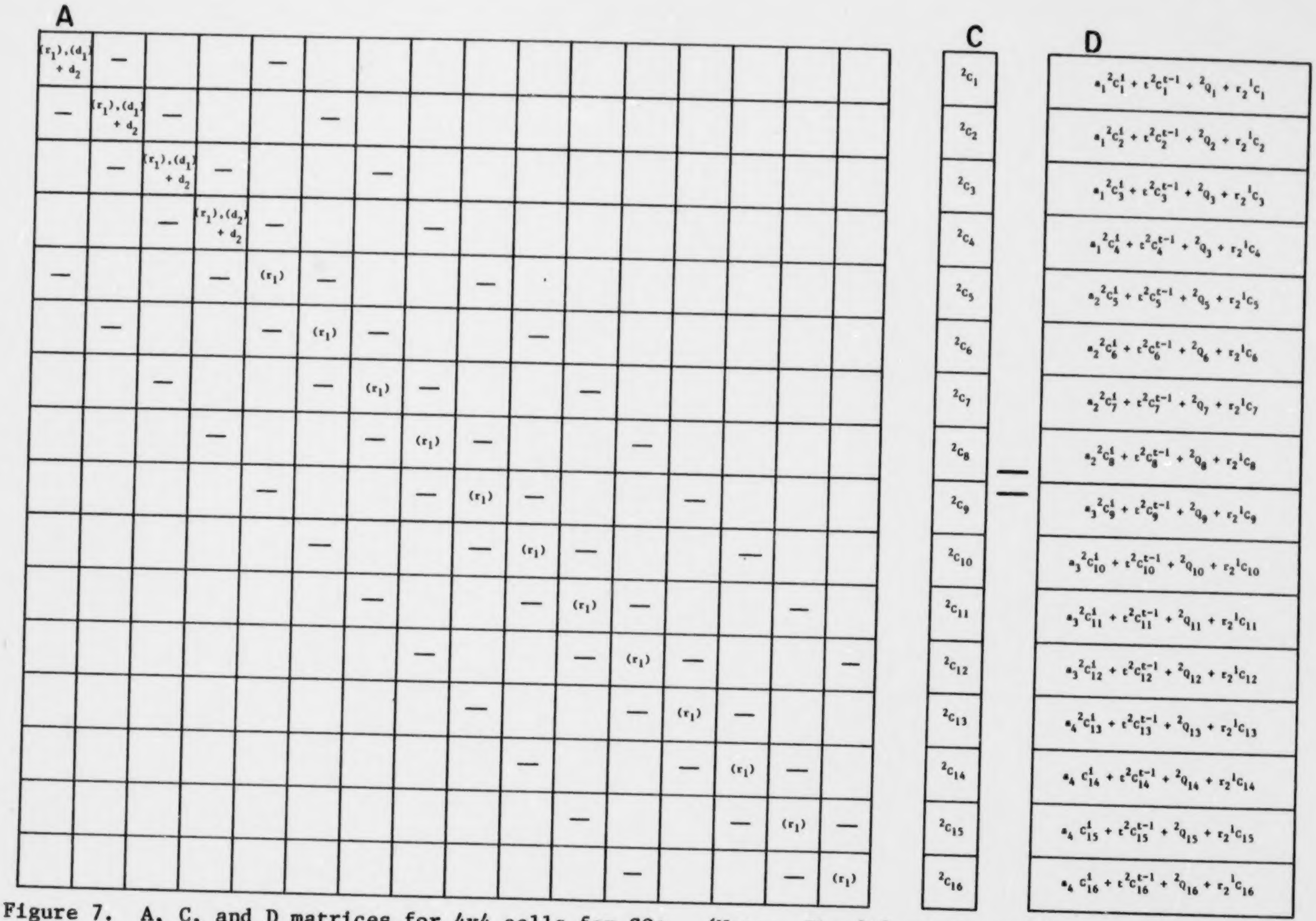
Example matrices for a 4x4 plane of cells are written out in full in Figures 6 and 7 using the abbreviations defined on pages 33 and 34.

SUMMARY OF THEORY

The steps in the SO_2 and SO_4 equation formulation from the differential microscale to the regional macroscale are briefly summarized. Starting from specific conservation of mass equations for SO_2 and SO_4 for an infinitesimal volume element which includes the processes of wind transport, turbulent diffusion, chemical reactions and source input the path has been traced to the matrix formulation which permits concentration calculations over a finite three-dimensional region. The initial equations, called the Model Differential Equations, were reformulated for a finite volume element (cell) into the Model SO_2/SO_4 Finite Difference Equations. Initial and boundary conditions were selected. The finite difference form was then cast into a multi-cell or matrix form permitting simultaneous solution of equations for an entire plane of cells. This is the basic unit of calculation used to solve for the concentrations in the region. The method of solution for the entire regional network proceeds as follows: the simultaneous finite difference equations together with initial and boundary conditions have been cast in matrix form for all cells within a yz-plane for one time-step; the concentrations for all cells within that plane can be solved for as represented in the matrix solution [C] = [D]/[A]; this single plane, single time interval solution is carried out first for each time-step for a given plane for a 1 hr period, then for the next downwind plane for the same hour, then for the next plane, etc., until all planes and hence all cells within the region have been solved for a given hour. The end result is a concentration value for each cell at the end of the hour. New meteorological data is input for the next hour and the cycle repeated. It is repeated over and over for each hour for each and every cell until the end of the simulation period.

$$
\overset{\textbf{A}}{\begin{bmatrix}
a_1+\varepsilon+r_1+e_1+f_{3/2}+d_1 & -e_1 & & & -f_{3/2} & & & & & & & & & & & \\
-e_1 & a_1+\varepsilon+r_1+2e_1+f_{3/2}+d_1 & -e_1 & & & -f_{3/2} & & & & & & & & & & \\
 & -e_1 & a_1+\varepsilon+r_1+e_1+f_{3/2}+d_1 & -e_1 & & & -f_{3/2} & & & & & & & & & \\
 & & -e_1 & a_1+\varepsilon+r_1+2e_1+f_{3/2}+d_1 & & & & -f_{3/2} & & & & & & & & \\
-f_{3/2} & & & & a_2+\varepsilon+r_1+e_2+f_{5/2}+f_{3/2} & -e_2 & & & -f_{5/2} & & & & & & & \\
 & -f_{3/2} & & & -e^2 & a_2+\varepsilon+r_1+2e_2+f_{5/2}+f_{3/2} & -e_2 & & & -f_{5/2} & & & & & & \\
 & & -f_{3/2} & & & -e_2 & a_2+\varepsilon+r_1+2e_2+f_{5/2}+f_{3/2} & -e_2 & & & -f_{5/2} & & & & & \\
 & & & -f_{3/2} & & & -e_2 & a_2+\varepsilon+r_1+e_2+f_{5/2}+f_{3/2} & & & & -f_{5/2} & & & & \\
 & & & & -f_{5/2} & & & & a_3+\varepsilon+r_1+e_3+f_{7/2}+f_{5/2} & -e_3 & & & -f_{7/2} & & & \\
 & & & & & -f_{5/2} & & & -e_3 & a_3+\varepsilon+r_1+2e_3+f_{7/2}+f_{5/2} & -e_3 & & & -f_{7/2} & & \\
 & & & & & & -f_{5/2} & & & -e_3 & a_3+\varepsilon+r_1+2e_3+f_{7/2}+f_{5/2} & -e_3 & & & -f_{7/2} & \\
 & & & & & & & -f_{5/2} & & & -e_3 & a_3+\varepsilon+r_1+e_3+f_{7/2}+f_{5/2} & & & & -f_{7/2} \\
 & & & & & & & & -f_{7/2} & & & & a_4+\varepsilon+r_1+e_4+f_{7/2} & -e_4 & & \\
 & & & & & & & & & -f_{7/2} & & & -e_4 & a_4+\varepsilon+r_1+2e_4+f_{7/2} & -e_4 & \\
 & & & & & & & & & & -f_{7/2} & & & -e_4 & a_4+\varepsilon+r_1+2e_4+f_{7/2} & \\
 & & & & & & & & & & & -f_{7/2} & & & -e_4 & a_4+\varepsilon+r_1+e_4+f_{7/2}
\end{bmatrix}}
\overset{\textbf{C}}{\begin{bmatrix}
{}^1C_1 \\ {}^1C_2 \\ {}^1C_3 \\ {}^1C_4 \\ {}^1C_5 \\ {}^1C_6 \\ {}^1C_7 \\ {}^1C_8 \\ {}^1C_9 \\ {}^1C_{10} \\ {}^1C_{11} \\ {}^1C_{12} \\ {}^1C_{13} \\ {}^1C_{14} \\ {}^1C_{15} \\ {}^1C_{16}
\end{bmatrix}}
=
\overset{\textbf{D}}{\begin{bmatrix}
a_1\,{}^1C_1^t+\varepsilon\,{}^1C_1^{t-1}+{}^1Q_1 \\
a_1\,{}^1C_2^t+\varepsilon\,{}^1C_2^{t-1}+{}^1Q_2 \\
a_1\,{}^1C_3^t+\varepsilon\,{}^1C_3^{t-1}+{}^1Q_3 \\
a_1\,{}^1C_4^t+\varepsilon\,{}^1C_4^{t-1}+{}^1Q_4 \\
a_2\,{}^1C_5^t+\varepsilon\,{}^1C_5^{t-1}+{}^1Q_5 \\
a_2\,{}^1C_6^t+\varepsilon\,{}^1C_6^{t-1}+{}^1Q_6 \\
a_2\,{}^1C_7^t+\varepsilon\,{}^1C_7^{t-1}+{}^1Q_7 \\
a_2\,{}^1C_8^t+\varepsilon\,{}^1C_8^{t-1}+{}^1Q_8 \\
a_3\,{}^1C_9+\varepsilon\,{}^1C_9^{t-1}+{}^1Q_9 \\
a_3\,{}^1C_{10}^t+\varepsilon\,{}^1C_{10}^{t-1}+{}^1Q_{10} \\
a_3\,{}^1C_{11}^t+\varepsilon\,{}^1C_{11}^{t-1}+{}^1Q_{11} \\
a_3\,{}^1C_{12}^t+\varepsilon\,{}^1C_{12}^{t-1}+{}^1Q_{12} \\
a_4\,{}^1C_{13}^t+\varepsilon\,{}^1C_{13}^{t-1}+{}^1Q_{13} \\
a_4\,{}^1C_{14}^t+\varepsilon\,{}^1C_{14}^{t-1}+{}^1Q_{14} \\
a_4\,{}^1C_{15}^t+\varepsilon\,{}^1C_{15}^{t-1}+{}^1Q_{15} \\
a_4\,{}^1C_{16}^t+\varepsilon\,{}^1C_{16}^{t-1}+{}^1Q_{16}
\end{bmatrix}}
$$

Figure 6. A, C, and D matrices for 4x4 cells for SO_2. (Note: Any cell without a symbol has a zero value.)



A

$(r_1),(d_1) + d_2$	—			—											
—	$(r_1),(d_1) + d_2$	—			—										
	—	$(r_1),(d_1) + d_2$	—			—									
		—	$(r_1),(d_2) + d_2$	—			—								
—			—	(r_1)	—			—							
	—			—	(r_1)	—			—						
		—			—	(r_1)	—			—					
			—			—	(r_1)	—			—				
				—			—	(r_1)	—			—			
					—			—	(r_1)	—			—		
						—			—	(r_1)	—			—	
							—			—	(r_1)	—			—
								—			—	(r_1)	—		
									—			—	(r_1)	—	
										—			—	(r_1)	—
											—			—	(r_1)

C		D
${}^2c_1$		$a_1{}^2c_1^t + t^2c_1^{t-1} + {}^2Q_1 + r_2{}^1c_1$
${}^2c_2$		$a_1{}^2c_2^t + t^2c_2^{t-1} + {}^2Q_2 + r_2{}^1c_2$
${}^2c_3$		$a_1{}^2c_3^t + t^2c_3^{t-1} + {}^2Q_3 + r_2{}^1c_3$
${}^2c_4$		$a_1{}^2c_4^t + t^2c_4^{t-1} + {}^2Q_3 + r_2{}^1c_4$
${}^2c_5$		$a_2{}^2c_5^t + t^2c_5^{t-1} + {}^2Q_5 + r_2{}^1c_5$
${}^2c_6$		$a_2{}^2c_6^t + t^2c_6^{t-1} + {}^2Q_6 + r_2{}^1c_6$
${}^2c_7$		$a_2{}^2c_7^t + t^2c_7^{t-1} + {}^2Q_7 + r_2{}^1c_7$
${}^2c_8$	=	$a_2{}^2c_8^t + t^2c_8^{t-1} + {}^2Q_8 + r_2{}^1c_8$
${}^2c_9$		$a_3{}^2c_9^t + t^2c_9^{t-1} + {}^2Q_9 + r_2{}^1c_9$
${}^2c_{10}$		$a_3{}^2c_{10}^t + t^2c_{10}^{t-1} + {}^2Q_{10} + r_2{}^1c_{10}$
${}^2c_{11}$		$a_3{}^2c_{11}^t + t^2c_{11}^{t-1} + {}^2Q_{11} + r_2{}^1c_{11}$
${}^2c_{12}$		$a_3{}^2c_{12}^t + t^2c_{12}^{t-1} + {}^2Q_{12} + r_2{}^1c_{12}$
${}^2c_{13}$		$a_4{}^2c_{13}^t + t^2c_{13}^{t-1} + {}^2Q_{13} + r_2{}^1c_{13}$
${}^2c_{14}$		$a_4\ c_{14}^t + t^2c_{14}^{t-1} + {}^2Q_{14} + r_2{}^1c_{14}$
${}^2c_{15}$		$a_4\ c_{15}^t + t^2c_{15}^{t-1} + {}^2Q_{15} + r_2{}^1c_{15}$
${}^2c_{16}$		$a_4\ c_{16}^t + t^2c_{16}^{t-1} + {}^2Q_{16} + r_2{}^1c_{16}$

Figure 7. A, C, and D matrices for 4x4 cells for SO4. (Note: The [A] matrix is identical to that for SO_2 (Figure 6), as indicated by "-" except on the diagonal where the symbols in parentheses are to be deleted and those not in parentehses are to be added).

DISCUSSION OF SIMULATION SEQUENCE

So far the general theory for finding the cell-by-cell concentrations has been discussed. Now an outline discussion is given of how the theory is carried out within the main computer program, UWATM-SOX. This will acquaint the user with the actual sequence of program execution. Details on how to run the program are given in Sections 12 and 13.

The program begins by reading in from mass storage the emissions data. It is assumed to be single-valued and constant over the time period of simulation.

Next, the hourly calculations are begun by reading in the first hour's meteorological data from mass storage. This read-in statement marks the top of the large loop for all calculations carried out hourly.

Next, the plume rise is calculated for each source for the hour and it is determined if lofting occurs. If it does a new value of the mixing height is assigned.

Next, the Δz dimension of the variable-sized vertical cells is determined from the input (or reassigned) mixing height for the hour and the user-specified number cells.

Next, given the vertical cell structure and input meteorological data, the wind and diffusivity profiles for the hour are calculated, and, if the lofting condition has occurred for any source, the lateral and vertical diffusivities above the old mixing height are zeroed, thus "trapping" the pollutants within a downwind line of cells since only wind transport is thus allowed for.

Next, the deposition velocity for the hour is calculated from input data and the 1-m wind calculated from the wind profile equations.

Next, the grid coordinates of each source are rotation transformed from the fixed grid system to the rotating system. (The dual fixed and rotating cell systems have only been alluded to in Section 2, they are explained in Sections 11 and 12, suffice it to say that the fixed system is the user-created grid network and the rotating system rotates so that the x-direction is always parallel with the wind vector and is the system in which all the calculations are performed.) The emissions are placed in the vertical cell within which each source's effective stack height lies.

Next, the A-matrix is constructed for the hour from the wind speed, vertical and lateral diffusivities values for each cell, chemical reaction parameters, deposition velocity, cell dimensions and time interval of calculation. Two A-matrices are constructed for SO_2 and for SO_4.

Next is begun the x-step (downwind) loop for the region starting with the leading upwind plane of NUMY*NUMZ cells.

Next is begun the t-step (time interval within 1 hr) loop starting at the beginning of an hour.

Next, the D-matrix is constructed for SO_2 for a given x-step and given t-step from a knowledge of the previous x-step concentrations for the current t-step, previous t-step concentrations for the current x-step and the emission rates of sources within the given x-step.

Next, the SO_2 concentrations are solved for the given x-step and given t-step.

Next, the D-matrix is constructed for SO_4 from the now known SO_2 concentrations. The SO_4 concentrations are solved for the same x-step and same t-step as for the SO_2.

The above three steps are now repeated for all (NUMT) t-steps for the given x-step.

Next, all concentrations for the given x-step are transferred from the rotating system to the fixed system for storage.

The above four steps are now repeated for all (NUMX) x-steps for the region for the given hour.

Next, the ground level concentrations for the region are picked off (from the lowest level cells of the fixed system) and stored.

Next, the dry deposition fluxes are calculated from the ground level concentrations. (Note: this calculation is not a duplication of the dry deposition calculations within the above loops. It is done this way because within the loops all processes (wind, diffusion, chemical, deposition) are solved for simultaneously and the impact of a single process cannot be extracted on a cell-by-cell basis.)

Next, the wet deposition fluxes are calculated. This calculation, because of the nature of the theory involved (see Section 8), is done outside the main equations. Instead of wet deposition being considered on a cell-by-cell basis an entire vertical column of cells is considered at once.

Next, selected hourly information is stored on tape.

This ends the processing sequence for a 1 hr period. It now starts over again with the reading in of the next hour's meteorological data. The whole pattern is repeated over and over until all the hours in the time period of simulation have been completed.

SECTION 7

WIND AND DIFFUSIVITY PROFILES

The wind transport and turbulent diffusion processes affecting pollutant behavior are approximated in the atmospheric boundary layer by a set of horizontal wind speed, lateral diffusivity, and vertical diffusivity profiles.

With regards to the motion of the air, the atmosphere can be segmented vertically into two major layers--the atmospheric (or planetary) boundary layer from the ground to roughly 300 to 1000 m in which the effects of the earth's surface are felt, and a geostropic layer above it in which the motion of the air approximates a nonviscous fluid and the flow is influenced only by horizontal pressure gradients and Coriolis forces. In air pollution modeling on a micro- and meso-scale the atmospheric boundary layer is the most important and is the sole concern of this model. The geostropic layer is important on a macro- or global-scale.

The atmospheric boundary layer can be divided into two regions--a surface layer extending from the ground to roughly 50 to 100 m in which the shear stress and heat flux are assumed constant and the air motion is determined primarily by the nature of the surface and the vertical temperature gradient, and a layer between the surface layer and geostropic layer in which the shear stress and heat flux are variable and the air motion is determined by the surface drag, temperature gradient, and Coriolis forces. In the model these two regions are characterized by a different set of equations. Figure 8 shows the general character of the profiles.

The model assumes that the mixing height (as derived from the NCC tape) marks the top of the atmospheric boundary layer and is where the wind reaches geostrophic equilibrium between the horizontal pressure gradient and Coriolis forces. The height of the layer changes hourly.

The model simplifies the complex dependence of the profiles on heat flux, temperature gradient, etc. by using the stability concept and classifying the profile equations into three categories for stable, unstable, and neutral stabilities. The hourly stability is part of the meteorological data-base (see Section 5) and depending on the value one of the three categories of profile equations is chosen for calculation for the hour. The collection of equations is shown in Table 6 based on the following theory:

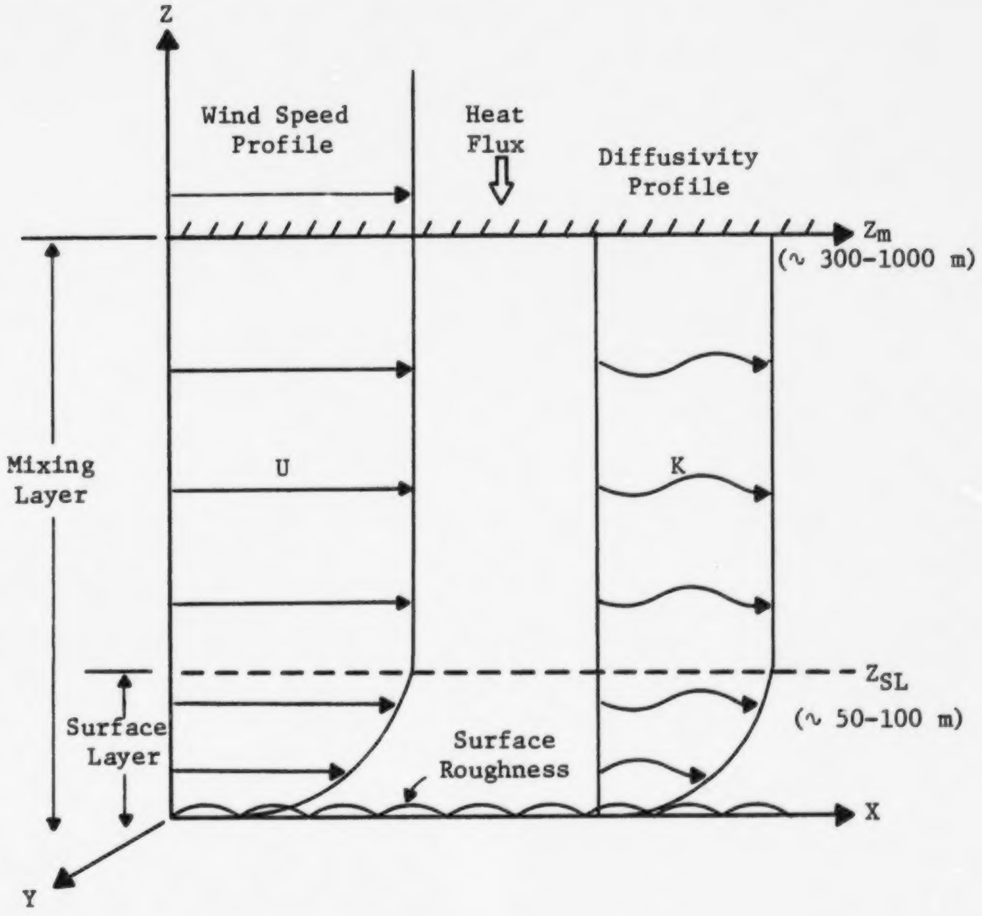

Z
Wind Speed Profile
Heat Flux
Diffusivity Profile
Z_m
(∿ 300-1000 m)
Mixing Layer
U
K
Z_{SL}
(∿ 50-100 m)
Surface Layer
Surface Roughness
X
Y

Figure 8. Wind and diffusivity profiles.

TABLE 6. WIND AND DIFFUSIVITY PROFILE EQUATIONS

Stability	z_{max}	Wind Speed, u	Vertical Eddy Diffusivity, K_z	Lateral Eddy Diffusivity, K_y
Neutral	$400u_*$	$\frac{u_*}{0.4} \ell n(\frac{z+z_o}{z_o})$	$0.4u_*z$	EDDYN * ^NK_z
Stable	L	$\frac{u_*}{0.4}[\ell n(\frac{z+z_o}{z_o})+ \frac{5.2z}{L}]$	$0.4u_*z/(1 + \frac{5.2}{L}z)$	EDDYS * ^SK_z
	6L	$\frac{u_*}{0.4}[\ell n(\frac{z+z_o}{z_o}) + 5.2]$	$0.4u_*z/6.2$	
Unstable	2L	$\frac{u_*}{0.4}[2(\tan^{-1}x-\tan^{-1}x_o) + \ell n(\frac{x-1}{x_o-1})-\ell n(\frac{x+1}{x_o+1})]$ $x = [1-15(z+z_o)/L]^{0.25}$ $x_o = (1-15z_o/L)^{0.25}$	$0.4u_*z(1 - \frac{15z}{L})^{.25}$	EDDYU * ^UK_z
Neutral	z_m	$(u_g-u_{SL}) (\frac{z-400u_*}{z_m-400u_*})^{0.2} + u_{SL}$	$0.4u_*(400u_*)$	EDDYN * ^NK_z
Stable	z_m	$(u_g-u_{SL}) (\frac{z-6L}{z_m-6L})^{0.5} + u_{SL}$	$0.4u_*(L)$	EDDYS * ^SK_z
Unstable	z_m	$(u_g-u_{SL}) (\frac{z+2L}{z_m+2L})^{0.2} + u_{SL}$	$0.4u_*(400u_*) (1 - \frac{6000u_*}{L})^{0.25}$	EDDYU * ^UK_z

SURFACE LAYER

The surface layer profiles are based on the similarity theory of Monin-Obukhov (1954). The stability is characterized by the parameter L.

$$L = - \frac{u_*^3 \rho \hat{C}_p T_a}{kgH} \tag{12}$$

where L is Monin-Obukhov Length

u_* is friction velocity

ρ is ambient air density

$\hat{C}_p$ is heat capacity at constant pressure/unit mass of air

T_a is ambient air temperature

k is Karman's constant

g is gravitational acceleration

H is vertical mean turbulent heat flux

The friction velocity can be expressed as a function of a drag coefficient acting on the geostrophic wind:

$$u_* = C_g U_g \tag{13}$$

The drag coefficient can be expressed empirically as a function of the surface Rossby number. The following formula is from Lettau (1959) and applies to a neutral atmosphere.

$$C_g^N = \frac{0.16}{\log_{10}(R_o) - 1.8} \tag{14}$$

where C_g^N is drag coefficient for neutral atmosphere

R_o, the Rossby number is $\frac{U_g f}{z_r}$

U_g is geostrophic wind

f is Coriolis parameter

z_r is surface roughness

The above drag coefficient for a neutral atmosphere is applied to non-neutral atmospheric conditions using the following scheme.

$$\text{Unstable: } C_g = 1.2\, C_g^N \tag{15}$$

$$\text{Stable: } C_g = 0.6\, C_g^N \tag{16}$$

The L-parameter is thus completely determined by the above equations if the following variables are known: surface roughness (z_r), Coriolis parameter (f), geostrophic wind (U_g), heat flux (H), gravitational acceleration (g), Karman's constant (k), air temperature (T_a), specific heat of air ($\hat{C}_p$) and air density (ρ). The following are given constant values: $f = 10^{-4}$, $g = 9.8\ \text{m/sec}^2$, $k = 0.4$, $\hat{C}_p = 1.012$ kJ/kg °C (at 20°C and standard pressure) $\rho = 1.204\ \text{kg/m}^3$ (at 20°C and standard sea level pressure) and a single value is given to z_r depending on the region of model application. Therefore to calculate hourly variations in L hourly variations of geostrophic wind, heat flux and air temperature need to be known. The heat flux and air temperature are part of the hourly data-base and the geostrophic wind is internally calculated within a subroutine of the main UWATM-SOX program each hour using an iteration scheme based on a knowledge of the surface wind speed and height at which it was measured.

Surface Layer Wind

From the Monin-Obukov (1954) theory the velocity gradient in the vertical is given by

$$\frac{\partial u}{\partial z} = \frac{u_* \phi_M}{kz} \tag{17}$$

where ϕ_M is a function of Z/L as follows:

Neutral: $Z < ku_* f$ $\quad \phi_M = 1$

Unstable: $-2 < Z/L < 0$ $\quad \phi_M = (1 - 15\frac{Z}{L})^{0.25}$

Stable: $0 < Z/L < 1$ $\quad \phi_M = 1 + \alpha\frac{Z}{L}$

$1 < Z/L < 6$ $\quad \phi_M = 1 + \alpha$

where $\alpha = 5.2$ (Webb 1970)

If the velocity gradient is integrated from Z_r to $Z + Z_r$ (where technically Z is measured starting from the surface roughness height but for all practical purposes can be assumed to be measured from ground level), and the integration is carried out for each of the four above stability conditions then the surface layer wind speed equations in Table 6 are obtained.

Surface Layer Diffusivity

The vertical turbulent eddy diffusivities are assumed equal to the vertical turbulent momentum diffusivities. The latter may be defined in terms of the shear stress:

$$\tau/\rho = K_M \left(\frac{\partial u}{\partial z} \right) \tag{18}$$

where τ is atmospheric shear stress
ρ is atmospheric density
K_M is momentum diffusivity or eddy viscosity
$\frac{\partial u}{\partial z}$ is vertical wind velocity gradient

Recalling that

$$u_*^2 = \tau_o/\rho, \tag{19}$$

where τ_o is the shear stress at the surface

and making the common assumption that the shear stress is constant within the surface layer, the vertical momentum diffusivity can be expressed by:

$$K_M = u_*^2 \Big/ \frac{\partial u}{\partial z} . \tag{20}$$

If the previously given expression for the velocity gradient and the ϕ_M functions are substituted into the above equation the surface layer eddy diffusivities (K_z) in Table 6 are obtained.

ABOVE SURFACE LAYER WIND AND DIFFUSIVITY

The wind speed equations above the surface layer are a form of the commonly used empirical power-law:

$$U = (U_g - U_{SL}) \left(\frac{Z - Z_{SL}}{Z_m - Z_{SL}} \right)^P + U_{SL} . \tag{21}$$

where Z_{SL} is height of surface layer
Z_M is mixing height
U_g is geostrophic wind speed (i.e., wind speed at mixing height)
U_{SL} is wind speed at Z_{SL}
p is empirically-derived exponent which depends on stability.

From measurements on wind profiles (Jones 1971) the following model values for p are derived.

Neutral: $p = 0.2$
Unstable: $p = 0.2$
Stable: $p = 0.2 + |\text{heat flux}|$

For the diffusivity, the model assumes it is constant and is the value at the top of the surface layer as determined from the surface layer equations. The height of the surface layer is set as follows.

$$\text{Neutral:} \quad Z_{SL} = 0.1 \frac{ku_*}{f} \tag{22}$$

$$\text{Unstable:} \quad Z_{SL} = 0.1 \frac{ku_*}{f} \tag{23}$$

$$\text{Stable:} \quad Z_{SL} = 6L \tag{24}$$

If these Z-values are substituted into the previously defined K_z-values, the K_z eddy diffusivity equations in Table 6 are obtained.

LATERAL DIFFUSIVITY

The lateral eddy diffusivity is in all cases assumed to be constantly proportional to the vertical diffusivity. It is a user-supplied constant multiple of the vertical diffusivity value. The user assigns a constant for each stability category (called EDDYN, EDDYS, EDDYU for neutral, stable, and unstable, respectively) and the K_z-value is multiplied by this constant. For model applications the constants have ranged from 1 (for 10's of km scale) to 100 (100's of km scale). For help in selecting values see references (Heffter 1965, Pasquill 1974, Randerson 1972).

SUMMARY OF THEORY

The wind and diffusivity profiles are calculated for two regions in the atmospheric (planetary) boundary layer, one above and one below the surface layer height. The surface layer profiles of wind speed and vertical diffusivity are calculated from the Monin-Obukhov (1954) similarity theory. The above surface layer profile for the wind speed is a form of the empirical power-law and for the vertical diffusivity is assumed constant. Three sets of equations are derived for each profile for neutral, unstable, and stable conditions. In all, there are seven different wind speed equations and seven vertical diffusivity equations for the two regions. In all cases the lateral diffusivity is a user-supplied constant multiple of the vertical diffusivity.

To calculate the profiles the following variables need to be known:

1. Geostrophic wind (U_g)
2. Heat flux (H)
3. Ambient air temperature (T_a)
4. Surface roughness (Z_r)
5. Mixing height (Z_M)
6. Lateral diffusivity multipliers (EDDYN, EDDYS, EDDYU)
7. Coriolis parameter (f), gravitational constant (g), Karman's constant (k), specific heat of air ($\hat{C}_p$), air density (ρ), alpha

(α), power-law exponents for neutral, stable and unstable conditions (p).

The last set (7.) are assigned constant values within the program but they can be user altered if desired. The surface roughness and lateral diffusivity constants are user-supplied constants appropriate to the regional terrain and scale of application. The heat flux, air temperature and mixing height are part of the hourly meteorological data-base. The geostrophic wind is internally calculated in the profile subroutine.

DISCUSSION OF PROGRAMMING SEQUENCE

This is an outline discussion of the sequence of program execution in the wind and diffusivity profiles subroutine (WINDIF).

First, the upper or geostrophic wind (assumed to be the wind speed at the mixing height) is estimated using a Modified Regula Falsi iteration technique. Starting from only a knowledge of the surface wind speed (known hourly from the meteorological data-base) and the height at which it was measured (assumed in the program to be 10 m), and using the form of wind profile equations already discussed the wind speed at the mixing height is found. The iteration technique is very efficient usually using 3 to 5 iterations to find the upper wind speed within 0.5 m/sec.

Next, the values of u, K_z, K_y are calculated for the given vertical cell structure. For each cell u and K_y are found at the center, and K_z at the top and bottom. If there are six cells in the vertical, the profiles will consist of six wind speeds, six lateral diffusivities, and four vertical diffusivities (the ground level and mixing height values are taken care of in the boundary conditions).

In the process of calculating the wind speed profile, the wind speed at 1 m off the ground is calculated. This is used in the deposition velocity calculation.

Next, the vertical mean wind is calculated. Though this is not directly used elsewhere in the model it is a useful characterization of the wind condition in the atmospheric boundary layer for the hour and its value is stored on tape.

Next, if lofting occurs (as determined by a previous comparison of point source plume rise to mixing height, and where, if the plume is above it, the mixing height has been reset to the 10 m above the old height) then all vertical and lateral diffusivities between the old and new mixing heights are set to zero thus effectively trapping all plumes above the old height within a single horizontal line of cells in which only the wind can move the pollutants as illustrated in Figure 9.

This ends the processing sequence for a 1 hr period. The profiles are assumed constant over the hour and are re-calculated for the next hour using new input.

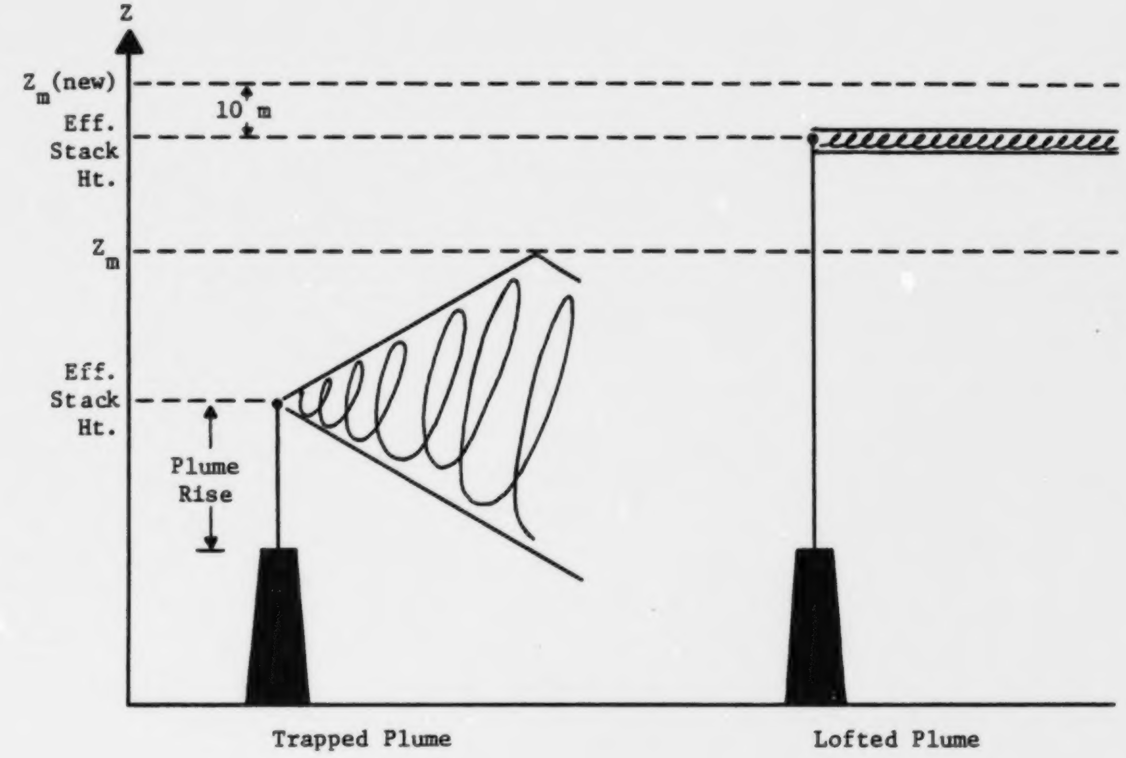

Z
Z_m(new)
10 m
Eff. Stack Ht.
Z_m
Eff. Stack Ht.
Plume Rise
Trapped Plume
Lofted Plume

Figure 9. Trapped and lofted plumes.

SECTION 8

DRY AND WET DEPOSITION SCHEMES

Dry and wet deposition are handled quite differently in the model. Dry deposition is handled by means of a deposition velocity. A portion of the pollutant located near the ground is deposited on the ground. In the model the pollutant flux is introduced as a ground level boundary condition to the solution of the SO_2 and SO_4 atmospheric dispersion equations. Wet deposition is handled by means of a theory (Scott 1978) in which the amount of pollutant removed and deposited is based on considering an entire vertical column of cells from ground to mixing height at once. The wet removal could be handled similar to the dry removal by using a washout coefficient applied to every cell and hence becoming part of the dispersion equation solutions, but as Scott (1978) argues it is not obvious that a first-order approximation is adequate for describing wet deposition. In the theory developed the wet removal rate is related to the surface level concentration and the precipitation rate.

DRY DEPOSITION

Dry deposition of gases such as SO_2 occurs by absorption and adsorption on vegetation, soil, surface water, etc. Dry deposition of particulates, such as particulate SO_4, occurs primarily by impaction onto surface materials. One of the simplest methods of quantifying the flux of any species is to multiply the concentration of that species near the ground by an effective deposition velocity as follows:

$$\text{Mass of dry deposition/unit area/unit time} = V_D C_g \qquad (25)$$

The deposition velocities are determined experimentally. They can be considered as functions of the meteorological conditions near the ground and the surface characteristics. The model uses an equation of the following form:

$$V_D = \frac{1}{r_a + r_s} \qquad (26)$$

where r_s is surface resistance

r_a is aerodynamic resistance is $\frac{u(1)}{u_*^2}$

$u(1)$ is wind speed at 1 m

u_* is friction velocity

The surface resistance (r_g) depends on the pollutant type and surface such as snow, water, vegetation, etc. The values are user-supplied appropriate for the region of application and form part of the input data. Some references discussing surface resistances include (Chamberlain 1966, Dovland and Eliassen 1976, McMahn and Denism 1979, Shepard 1974, Whelpdale and Shaw 1974, Husar et al. 1978). At present the model uses a separate summer and winter resistance for SO_2 and SO_4. The aerodynamic resistance (r_a) is internally calculated using information derived from the wind and diffusivity profiles subroutine. The deposition velocities are calculated hourly in the DEPVEL subroutine.

One assumption worth noting in the use of this method is that the ground level concentration used by the model is actually the average concentration in the first-level cell and depending on the Δz height of the first-level cell is not necessarily the concentration next to the earth's surface.

WET DEPOSITION

Only a sketch of the main elements of wet deposition theory is presented here. Several major assumptions are made. First, nucleation of cloud water droplets on SO_4 aerosols is the primary mechanism incorporating airborne SO_4 into the precipitation water. Second, dissolved SO_2 in the cloud droplets is in equilibrium with the atmospheric SO_2 concentration. Third, no in-cloud conversion from SO_2 to SO_4 takes place. Fourth, the Bergeron or cold cloud process is primarily responsible for precipitation development. This process assumes large relatively pollutant-free collector particles (snowflakes) sweep downward through the cloud accreting the cloud droplets (which contain the SO_2 and SO_4) and eventually fall to the ground as rain or snow.

The wet removal can be represented by the following differential equation:

$$\frac{d\overline{C}_n}{dt} = \frac{(jW)_Z - (jW)_{Z_o}}{Z - Z_o} \qquad (27)$$

where $\overline{C}_n$ is vertical average concentration of pollutant species n

j is precipitation rate (mass of water falling/unit area/unit time)

W is mass of pollutant/unit mass of precipitation water

$Z-Z_o$ is height of vertical column.

If j and W were known as functions of height it would be possible to incorporate this equation into the atmospheric dispersion equation, but this data is not available. The equation states that to know the wet removal the flux into and out of a vertical column must be known. The column is considered to extend from the ground to a height where the downward pollutant flux into it is nearly zero. It is assumed the in-coming pollutant flux is zero and the out-going flux is deposited on the ground. Scott's (1978) model expresses this situation mathematically.

The Bergeron process is illustrated in Figure 10. All four processes of rain and snow deposition of SO_2 and SO_4 will be characterized in a similar manner.

Large collector particles (snowflakes) enter the column from above and as they descend grow to larger size by accreting cloud droplets containing the dissolved SO_2 and nucleated SO_4 aerosol. The region of the cloud where precipitation growth is primarily by accretion of cloud droplets is called the riming zone. Since the snowflakes are assumed to be relatively pollutant free when they enter the riming zone, the wet downward pollutant flux at the top is assumed to be zero.

If the thickness of the riming zone can be determined and the distance between the ground and cloud base is known, than an estimate of the required $(Z-Z_o)$ vertical column can be made. If we assume:

1. The average fall speed of a median volume collector particle in the riming zone is $v_f = 3.89\ J^{0.10}$ (m/sec) where J is in mm/hr,
2. A residence time of 9 min for the particle in the riming zone, then, $\Delta Z_{rim} = 2100\ J^{0.10}$ (m).

If we further assume:

3. The distance from ground to cloud base is small compared to the approximate 2000 m riming zone,

then, $Z-Z_o \approx \Delta Z_{rim}$.

The wet removal rate equation can now be expressed as,

$$\frac{d\overline{C}_n}{dt} = -\frac{(jW)_{gnd}}{\Delta Z_{rim}} \qquad (28)$$

and if we incorporate the ΔZ_{rim} expression and convert units the following equation is derived:

$$\frac{d\overline{C}_n}{dt} = -\ 0.48\ J_G^{0.90}\ W_{G_n} \qquad (29)$$

where $\overline{C}_n$ is concentration of pollutant species n removed by wet deposition, averaged over the entire column from ground to top of riming zone (g/m^3)

J_G is precipitation rate measured at the ground (mm/hr)

W_{G_n} is pollutant mass/unit mass of precipitation water measured at the ground (g/g).

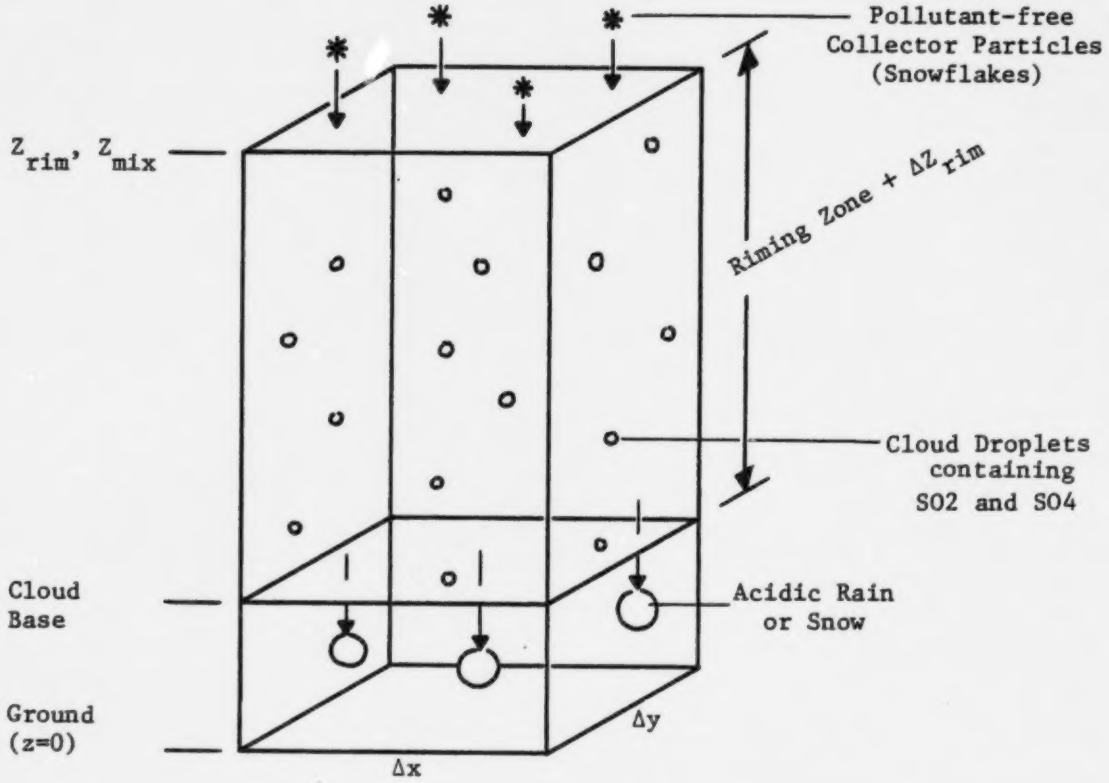

Pollutant-free Collector Particles (Snowflakes)
Z_{rim}, Z_{mix}
Riming Zone + ΔZ_{rim}
Cloud Droplets containing SO2 and SO4
Cloud Base
Acidic Rain or Snow
Ground (z=0)
Δy
Δx

Figure 10. Wet deposition scheme.

Therefore, all that is required to determine the wet removal rate for a species is the ground level precipitation rate and mass concentration of the pollutant in the precipitation water.

The following W_G-values are used in the model:

$$SO_4 \text{ rain or snow: } W_{G_{SO4}} = 0.46\ C_{G_{SO4}}\ J_G^{-\ 0.27} \tag{30}$$

$$SO_2 \text{ snow: } W_{G_{SO2}} = \beta\ \frac{C_{G_{SO2}}}{2}\ [1 - \exp(-2\overline{m})] \tag{31}$$

$$SO_2 \text{ rain: } W_{G_{SO2}} = \beta\ C_{G_{SO2}} \tag{32}$$

where C_G is ground level concentration

β is a correlation coefficient between the water dissolved SO_2 and the ambient ground level SO_2 concentrations is $= 10^{-2.0} + 0.75\ (pH - 3.9)$

pH is $-\log_{10} \left(\frac{2000\ W_{G_{SO4}}}{96} \right)$

$\overline{m}$ is cloud water concentration is $1.56 + 0.44\ \ell n\ J_G$.

These equations permit complete expression of the wet removal rates as functions of precipitation rate, ground level concentration and pH over the entire vertical column from ground to top of the riming zone (assumed equal to mixing height).

$$\left.\frac{\Delta\overline{C}_{SO_4}}{\Delta t}\right|_{\substack{\text{rain}\\ \text{or snow}}} = -0.22\ J_G^{0.63}\ C_{G_{SO_4}} \tag{33}$$

$$\left.\frac{\Delta\overline{C}_{SO_2}}{\Delta t}\right|_{\text{snow}} = -0.24\ J_G^{0.90}\ \beta\ C_{G_{SO_2}}\ (1 - \exp(-2\overline{m})) \tag{34}$$

$$\left.\frac{\Delta\overline{C}_{SO_2}}{\Delta t}\right|_{\text{rain}} = -0.48\ J_G^{0.90}\ \beta\ C_{G_{SO_2}} \tag{35}$$

Notice all expressions have the form:

$$\frac{d\overline{C}}{dt} = -KJ_G^a C_G\ . \tag{36}$$

This is not a first-order expression in $\overline{C}$ because of the dependence on the ground level concentration. If the ground level concentration is expressed in terms of a vertical average then it will be a first order expression. As a by-product of this theory the pH of the precipitation has been calculated.

All that is directly required to calculate the deposition is the ground level concentration and the precipitation rate. The precipitation rate is part of the hourly data-base and the ground level concentration has been previously calculated before the wet removal equations are solved. In the model application, the wet removal is determined for each vertical column of cells (there are a total of NUMX*NUMY columns in the region) for a 1 hr period. The Δt above is therefore 1 hr and the $\Delta\overline{C}$ is the vertical average pollutant mass/unit volume of air within a given column which is removed during the 1 hr period. All wet deposition operations are carried out in the WETDEP subroutine.

The model's computing sequence is such that the concentration for all cells in the region is calculated first, hence the ground concentration at the end of 1 hr is known, then applying the above formulas the concentration to remove from each column is found, this amount is subtracted from each cell in the column and done for all columns. The total mass/unit area wet deposited during 1 hr onto one of the horizontal grids is the sum for all cells of the removed concentration multiplied by the height of the cell. The total mass deposited on the region is the sum of the masses deposited on each grid.

SECTION 9

SO_2/SO_4 CHEMISTRY

The chemistry considered in the model primarily comes from data on coal-fired power plant plumes.

Most of the S in the combustion chamber of a coal-fired power plant is oxidized to SO_2, although a small percentage is oxidized to SO_3 and reacts with water vapor in the stack to form H_2SO_4. Approximately 2% of the S in SO_4 form goes up the stack (Forest and Newman 1977a and b). There is general agreement that SO_2 continues to react in the plume and forms sulfate aerosol as the plume diffuses (Gillani and Husar 1978, Schwartz and Newman 1978). Recent studies by Husar et al. (1978) showed that during noon hours the SO_2 conversion rate was 1 to 4%/hr, while the night conversion rate was below 0.5%/hr in the Labadie plume (from a 2400 MW coal-fired power plant near St. Louis).

Based on the above research the following chemical assumptions were made in the model.

1. SO_4 point source emissions are 2% of SO_2 emissions
2. Day-time SO_2-to-SO_4 conversion rate is 2%/hr
3. Night-time SO_2-to-SO_4 conversion rate is 0.5%/hr

The SO_4 emission percentage, though derived from coal-fired power plant data, is uniformly applied to all point sources independent of the nature of the source. The conversion rates, though derived from plume data, are applied uniformly throughout the region of study.

All of the mechanisms of SO_2 to SO_4 transformation are not known. Therefore, the model has assumed a strictly homogeneous and first-order conversion rate as explained in Section 6. The chemical reaction process is applied on a cell-by-cell basis for each time interval within a 1 hr period in the finite difference calculations.

SECTION 10

POINT SOURCES: PLUME RISE AND LOFTING

Pollutants upon entering the atmosphere from a point source stack are governed by buoyancy forces. Due to their momentum and temperature they rise in a plume above the stack. The plume rise process is usually such that the pollutants remain vertically coherent for varying heights and times before the atmosphere begins dispersing them. For most plume rise equations, it is assumed that the plume rises directly above the stack to a calculated height before disposal. Therefore the emissions are considered as originating at a point vertically located by an "effective stack height" (stack height plus plume rise).

The literature on plume rise equations is extensive and numerous formulas--both theoretical and empirical--have been proposed, none of which are satisfactory for all conditions. Generally, the factors affecting the rise are the meteorological and stack gas characteristics. The UWATM-SOX model uses a set of five equations distinguished according to heat emission rate from the stack and atmospheric stability. All five are empirical, having been derived from field measurements, and are based on the work of Moses and Carson (1968) and Briggs (1971). Table 7 lists the equations.

As seen from the Table 7, the non-constant variables are volumetric gas-flow rate (Q_v), stack gas temperature (T_s), ambient air temperature (T_a), wind speed at stack height (U_s), stack height (H_s), stack gas exit velocity (V_s) and stack diameter (D_s). From the point source emissions inventory one obtains: Q_v, T_s, H_s and D_s. From the meteorological database one obtained: T_a. The wind speed at stack height is calculated from an empirical power-law equation (as explained below) and the stack gas exit velocity is calculated from the formula given in the Table 7. Therefore all the needed data to calculate the plume rise is available in the user-created emissions and meteorological data files. No additional outside information is required.

Lofting is defined in the model as the condition where the plume rise exceeds the mixing height. This condition is important in the long-range transport of pollutants. The pollutants become trapped above the mixing layer for varying lengths of time and thus can be carried long distances before they reach ground level. This condition is accounted for in the model by a scheme in which, when lofting has occurred, the mixing height is artifically increased to just above the plume rise height. Then the lateral and vertical diffusivities are zeroed in the layer between the old and new mixing heights. This method effectively traps the plume within a horizontal "tube" of cells such that the pollutants can only be transported out of a

TABLE 7. PLUME RISE EQUATIONS

Heat flux	Stable	Neutral	Unstable
Hot source — $Q_H \geq 5000$ kcal/sec	$2.96 \left(\frac{Q_H}{U_s \frac{\Delta\Theta}{\Delta Z}} \right)^{1/3}$	$\frac{2.5\ Q_H^{1/3}\ H_s^{2/3}}{U_s}$	$\frac{2.5\ Q_H^{1/3}\ H_s^{2/3}}{U_s}$
Cool source — $Q_H < 5000$ kcal/sec	$\frac{-1.04\ V_s\ D_s + 4.58\ Q_H^{1/2}}{U_s}$	$\frac{.35\ V_s\ D_s + 5.41\ Q_H^{1/2}}{U_s}$	$\frac{3.47\ V_s\ D_s + 10.53\ Q_H^{1/2}}{U_s}$

where $Q_H \equiv$ heat emission rate from stack

$$= \frac{Q_v\ p\ m_a \hat{C}_p}{R} \left(\frac{T_s - T_a}{T_s} \right)$$

where $Q_v \equiv$ volume flow rate from stack

$p \equiv$ atmospheric pressure = 1.01325×10^5 Newtons/m^2

$m_a \equiv$ molecular weight of air = 28.797 g/mole of air

$R \equiv$ universal gas constant = 8.314 J/mole °K

$\hat{C}_p \equiv$ specific heat of air at constant pressure = 0.0003404 kcal/°K/gm

$T_s \equiv$ stack gas temperature (°K)

$T_a \equiv$ ambient air temperature (°K)

$U_s \equiv$ wind speed at stack height (m)

$\frac{\Delta\Theta}{\Delta Z} \equiv$ potential temperature gradient = 0.0064 °K/m

$H_s \equiv$ stack height (m)

$D_s \equiv$ stack inside diameter (m)

$V_s \equiv$ stack exit velocity of gases = $\frac{Q_v}{\Pi \left(\frac{D_s}{2} \right)^2}$

cell by the wind. The pollutants remain trapped as long as the plume rise, recalculated every hour, continues to puncture the mixing height. The scheme is illustrated in Figure 9.

PLUME RISE PROGRAMMING SEQUENCE

The plume rise calculation and the determination of lofting are carried out in the RISE subroutine. The sequence of steps is briefly explained.

First, the wind speed at stack height for each point source is calculated from the following equation:

$$U_s = U_o \left(\frac{H_s}{10}\right)^p \qquad (37)$$

where U_o is surface wind speed, obtained from meteorological data base, and assumed in the model to be measured at a height of 10 m above the ground

H_s is stack height

p is empirical exponent (values are given below for each Pasquill stability class--see pages 23 and 24 for stability discussion)

STABILITY	1	2	3	4	5	6	7
P	0.04	0.09	0.11	0.14	0.25	0.33	0.50

The stack height wind speed is not obtained from the wind profile subroutine because to incorporate lofting into the model it must be known before the WINDIF subroutine is executed. If lofting does occur WINDIF uses the new mixing height for calculating the profiles. Therefore, by introducing lofting into the model the wind and diffusivity profiles will, on those times when lofting occurs, be artificially altered because of the raising of the mixing height. It was felt justified to do this because of the relative infrequency of lofting but potential importance to long-range transport.

Next, the program calculates the plume rises for each source using one of the five equations depending on the source's heat flux and the stability condition.

Lastly, effective stack height is compared to the mixing height. If it is above, then the mixing height is reset 10 m above the effective stack height. For multiple sources the new mixing height is set just above the largest effective stack height. As discussed in the profile section, the diffusivities are zeroed for all cells between the old and new mixing heights.

This completes the RISE subroutine execution. The plume rise calculations for all sources and the lofting test are performed hourly with new input meteorological data.

SECTION 11

COMPUTER TECHNIQUES

In this section a few of the computer techniques most important to understanding the model are discussed:

1. Dual-grid system
2. Stop-start capability
3. Use of the "Fortran Procedure"
4. Tape storage of hour-by-hour calculations

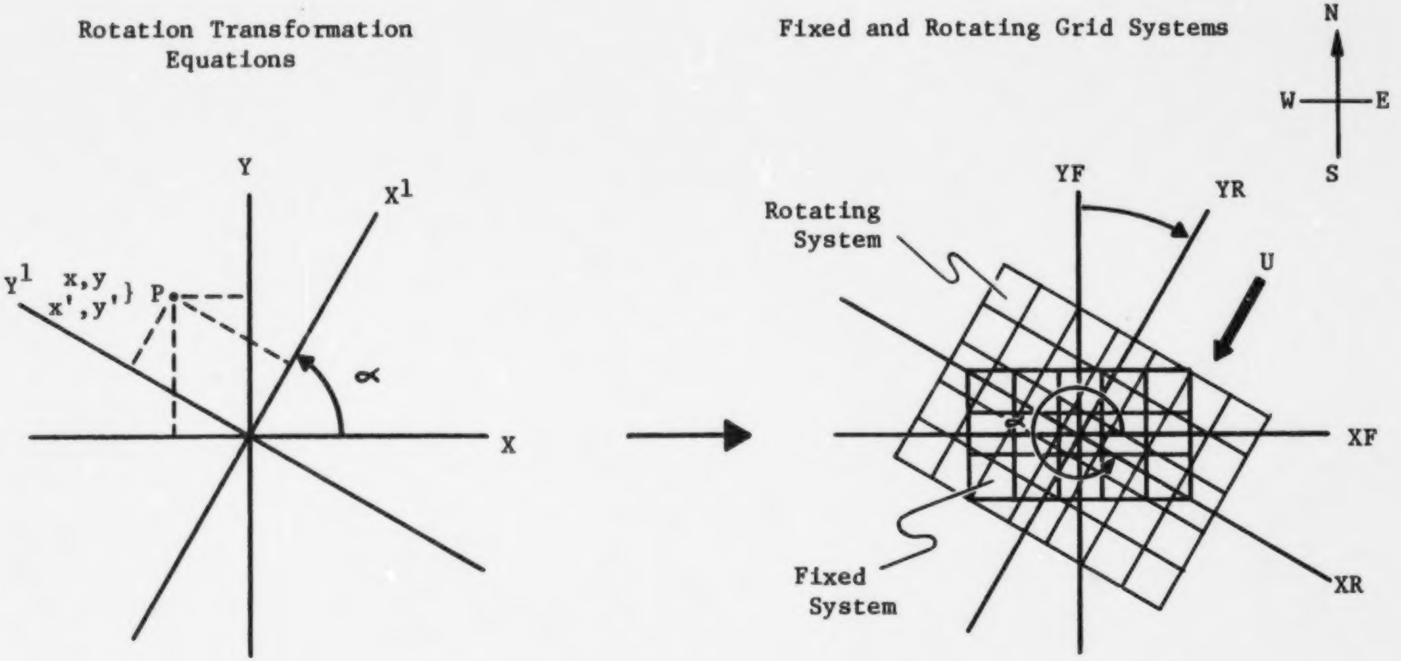
DUAL-GRID SYSTEM

The purpose of this scheme is to simulate constantly changing wind directions. It consists of using two grid systems overlapping with a common origin at their geographical center, one of which remains fixed in position and the other which rotates about the common origin. This is illustrated in Figure 11 on the next page.

It would be more accurate to call this a dual-cell system because the purpose is to transfer concentrations back and forth between the two 3D cell systems as the wind vector shifts. This should be kept in mind throughout the discussion whenever grid (implying 2D) is mentioned.

For a given region a grid pattern is selected. This will be the reference or fixed grid system. The difficulty of using only this grid for numerical calculations is that the wind transport is assumed to occur perpendicular to the cell face. Therefore, for any but the four cardinal wind directions a problem is posed. It is solved by overlapping the fixed system with another grid system which can freely rotate so that the upwind edge is always perpendicular to the wind vector. This is called the rotating system, and it is the system in which all the numerical calculations are performed. The fixed system then becomes the storehouse for the concentrations while the rotating system is being rotated at the end of each hour. The general procedure is to solve for the region's concentrations in the rotating system for a 1 hr period, then transfer them to the fixed system, then rotate the rotating system, then transfer the concentrations back into the rotating system and begin the calculations for the next hour. The continued back and forth transfers goes on hour after hour until the end of the simulation period.

The foundation of the scheme is the simple algebraic formula for rotation of coordinate axes. This is illustrated in Figure 11. For any



Rotation Transformation Equations
Y
X
X^1
Y^1
x,y
x',y'
P
∝
Fixed and Rotating Grid Systems
N
W
E
S
YF
YR
U
XF
XR
Rotating System
Fixed System
α

$x = x'\cos\alpha - y'\sin\alpha$
$y = x'\sin\alpha + y'\cos\alpha$

or

$x' = x\cos\alpha + y\sin\alpha$
$y' = -x\sin\alpha + y\cos\alpha$

x = XF
y = YF
x' = XR
y' = YR
α = -DIR
(DIR is direction from which wind blows.)

Figure 11. Dual grid system.

given point P, if the coordinates in a right-handed Cartesian coordinate system are known, then for any rotation of axes (assuming a common origin) through a given angle A the coordinates in the rotated system can be found with respect to the reference system. Remember that either pair of axes can be chosen as the reference pair, hence the two sets of equations. In the model these equations are used to find the centers of the grids in each system. This is used as the basis of determining which cell to transfer the concentrations to.

The scheme is basically complex bookkeeping and is not discussed further. Three subroutines employ the above technique--QTFM which rotates the emission coordinates, ROTFIX which transfers the concentrations from the rotating to fixed system and FIXROT which transfers them from the fixed to rotating.

STOP-START CAPABILITY

This refers to a procedure whereby the program may be terminated anywhere in the runstream and later started up again where it left off with no special requirements other than restarting the run. The way this is accomplished is to periodically during the runstream dump onto a mass storage file the essential data needed to start the program again. At the end of the selected dumping period (currently set for the end of each day) the file is rewritten. The contents of the file include: a stop-start flag, the date, the hour, some total mass information and all the SO_2 and SO_4 concentrations for the region as stored in the fixed system at the end of the selected dumping period.

If for any reason the main program (UWATM-SOX) runstream is terminated, all the necessary data is stored to restart it. When it is restarted it reads the contents of the stop-start file and proceeds the same as always. If the time period between dumps is say, a day, the program will not start exactly where it stopped but will start at the end of the nearest previous day. At most a day's information could be lost.

The only extra operation the capability imposes on the user is that at the beginning of a new run the stop-start file must be zeroed. A short deck described in Section 13 will do this.

THE FORTRAN PROCEDURE (PROC)

A FORTRAN procedure (PROC) is created by the Procedure Definition Processor (PDP) which is part of the SPERRY UNIVAC 1180 Series Executive System. The PROC generally consists of a set of statements which the programmer wants to use in more than one program and so creates a separate unit containing them. The set of statements in the FORTRAN PROC can be inserted into the source deck of any program with an INCLUDE statement.

In the model a FORTRAN PROC called APINFO has been created with two purposes in mind. First it contains most of the key PARAMETER and DIMENSION statements common to the main program and subroutines ensuring that if a change is made to one such statement it will be changed for all programs which use it. Second, it contains a set of EQUIVALENCE's to compactly store data in single-dimensioned arrays. This is a prerequisite for efficient tape storage of the hour-by-hour information.

TAPE STORAGE

The APINFO PROC creates a large single-dimensioned array also called APINFO in which is stored for every hour the date, some meteorological data, the wind and diffusivity profiles, some emissions data, total regional mass data, and ground level arrays for SO_2 and SO_4 concentrations, dry depositions and wet depositions. The APINFO array is written onto a user-supplied tape as a single record every hour. The tape output has been made flexible so that the wet deposition arrays are not written out unless it has rained or snowed during the input hour. This saves a large amount of otherwise "all zeros" tape space. At the end of the time period of simulation the tape is marked with a hardware end-of-file. Thus, if the simulation period were not a leap year, the tape file would consist of 8760 records. This file will be read and analyzed by the CDTAPE program as explained in Section 14.

SECTION 12

PROGRAM PREPARATION

Program Preparation is divided into three major steps.

1. Cell structure
2. Tape acquisition and file creation
3. Program changes

The first step involves creating the grid network to overlay the user's region of study and selecting the appropriate grid parameters. The second involves purchasing the tapes and creating the mass storage files for storing model-related information. The third involves the internal (program alteration and recompilation) and external (input data-deck) changes in each program. Each step is discussed separately.

CELL STRUCTURE

The general grid networks used in the model are illustrated in Figure 12 and will help to clarify the discussion.

There are nine parameters to select: DX,DY (the grid size); NUMXF, NUMYF (the fixed system number of grids); NUMX, NUMY (the rotating system number of grids), MGRID (the grid subdivision parameter), NBOXL (number of lower level fixed-height cells), and DZG (fixed height of lower level cells). The user will want to mark out the grids on the region of study and select the above seven parameters subject to the five conditions now to be explained.

The selection process is slightly complicated by five factors:

1. The grid ID numbering system does not correspond to a right-handed Cartesian coordinate system
2. The rotating grid system must be selected such that it completely overlaps the fixed system
3. A grid subdividing parameter (MGRID) must be selected
4. All grid parameters must be odd and
5. There are two classes of vertical cells, lower level fixed-height cells and upper level variable-height cells

The grid ID numbering starts in the upper-left (northeast) corner. The x-direction is in the Cartesian negative y-(southern) direction. The y-direction is in the Cartesian positive x-(eastern) direction. DX and DY follow this, not the Cartesian x and y directions. The reason for this

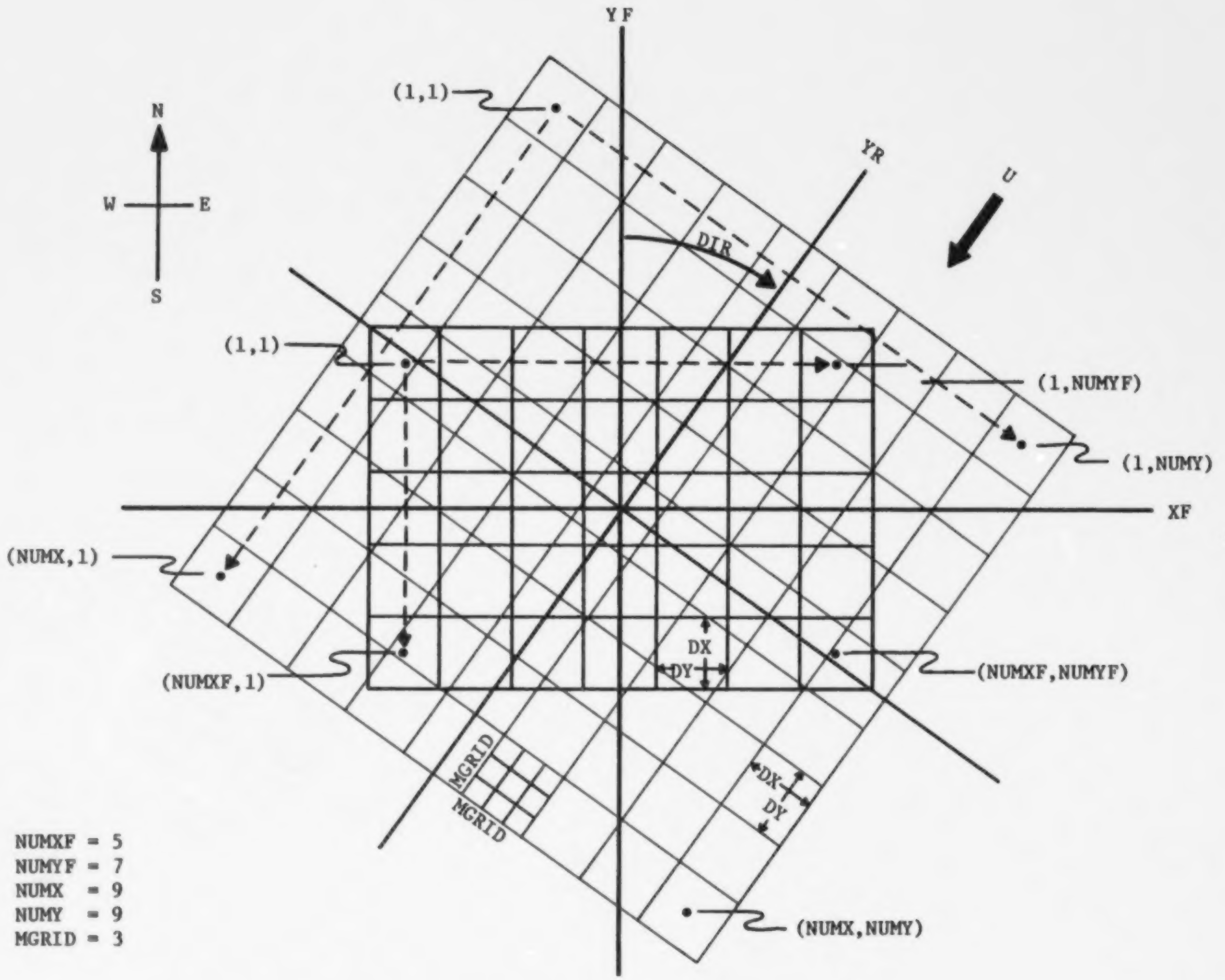

N
W
E
S
YF
XF
YR
U
DIR
(1,1)
(1,1)
(1,NUMYF)
(1,NUMY)
(NUMX,1)
(NUMXF,1)
(NUMXF,NUMYF)
(NUMX,NUMY)
DX
DY
DX
DY
MGRID
MGRID
NUMXF = 5
NUMYF = 7
NUMX = 9
NUMY = 9
MGRID = 3

Figure 12. Regional grid networks.

numbering system is to correspond to the conventional row-column matrix numbering schemes such that the x-direction is the downwind and y-direction is the crosswind direction. This simplifies the computer coding though it is confusing when trying to understand the bookkeeping behind the concentration transfer process.

The rotating system must be chosen to completely overlap the fixed system for all angles of rotation. The reason is that the internal program mass balance calculations assume this to be the case. If the overlap is not complete a consistent mass loss will occur during the calculations.

As seen in Figure 12, individual grids overlap to differing extents and/or overlap "empty space" outside the fixed system. A subdividing scheme is used to apportion the cell concentrations to be transfered according to the extent of overlap. (Remember the problem is to transfer concentrations between cells, so even though we continually speak of grids we mean cells.) Each grid (of either system depending if the transfer is from fixed to rotating or visa versa) is subdivided into a number of finer grids and the concentrations in the finer cells are transferred. The parameter MGRID will divide a larger grid into MGRID x MGRID subgrids. As many finer grids as computer cost and efficiency will allow can be used, but typically it wouldn't be more than five. The subgrids are not involved in the simulation, only the transfer process.

Finally, all grid parameters (NUMXF, NUMYF, NUMX, NUMY, MGRID) must be odd. This is because the rotation scheme assumes the origin of the Cartesian coordinate axes falls at the center of the center grid. For this to be true, the number of grids must be odd. There is no inherent reason even numbers couldn't be used, it is just that the computer code for this condition has not been created to date.

The above four conditions apply to the horizontal dimensioning. The fifth condition applies to the vertical dimensioning. There are two types of cells--lower level fixed-height and upper level variable-height. A specified number (NBOXL) of the lower level cells are fixed in height (DZG) and the remaining (NUMZ-NBOXL) upper level cells vary with changes in the mixing height $[\frac{ZM-(NBOXL*DZG)}{NUMZ-NBOXL}]$. Roughly, the cell-height dividing line corresponds to the surface layer division in the atmospheric boundary layer (see Section 7). This is the reason for the distinction.

TAPES AND FILES

Several tape and mass storage file tasks are required of the user. First, the user must create a program file. All programs for the University of Wisconsin-Madison modeling group are stored in the program file UWATM*ACIDRAIN. The user will want to copy this file into a new user-created program file with a different name. (It is called USER*PROGFILE in the remainder of the text.) This separate file is necessary because internal changes will have to be made to most of the programs to make them suited to the user's particular application. Second, the user will also want to create a mass storage file to contain the model-useable form of the emissions and meteorological data as produced by the MODEL-EMISS and METDATA programs. (It is called USER*EMISSMET in the following text.) Third, the user will need to create a file required for the stop-start capability. (It is called USER*STOPSTART in the text.) Fourth, the user will need to obtain a tape to contain the separate surface observations, mixing height and precipitation data files which are an intermediate step in the meteorological data processing. Fifth, the user will need to obtain tape(s) to contain the UWATM-SOX program's hourly output. The number required will depend on how many runs are to be made.

PROGRAM CHANGES

Upon completing these preliminary tasks of creating three mass storage files and obtaining at least two tapes, the user is set to begin preparing the programs to fit the specific application. This section describes how to prepare them for execution and Section 13 describes how to run the program. Program preparation involves two main tasks:

1. Internal program changes (altering and recompiling programs)
2. External program changes (making up data-decks)

Internal changes are made in the program source deck in certain PARAMETER, DATA, and FORMAT statements. The changes must be made through a "corrections deck" which alters the original program source deck and recompiles it. Every effort has been made to minimize internal changes but some cannot be avoided. External changes are made "outside" the programs through the input data-deck which can easily be altered for every program run. Most changes are made in this manner.

The format of the following discussion is to describe the internal changes and then the external changes for each and every program.

The form of the internal changes discussion is as follows. First, the correction run-cards are stated. These run-cards are the same no matter what program is being corrected, only the set of cards called the "corrections deck" is different. Next, the corrections deck for each program is listed and discussed change by change so it is clear what variables are being changed and how to find the appropriate values. These cards, once the user has filled in the designated values, are put with the run-cards to make a small corrections program. When executed it will alter and recompile the original program. When this is complete the program is ready for use.

The form of the external (data-deck) changes discussion is as follows. First the input READ statement(s) and FORMAT statement(s) (if any) "lifted" from the program are listed. Second, an example of each input card(s) is shown. Third, each value the user is required to supply is explained. Fourth, a brief comment on any relevant features of the input is given. The READ statements are discussed in the order in which the program executes them. Each statement is discussed separately. In the next section on program execution the data-deck as a whole is given. Note that the inputs discussed here are only those which require input cards to be typed.

It does not include the inputs from tape and mass storage because no additional work is required of the user other than executing the programs as given in the next section.

Sequence of Program Discussion

Emissions: PLUMEPOT
MODEL-EMISS

Met data: SFCOBSDATA
MIXINGHTDATA
PRECIPDATA
METDATA

Main program: APINFO
UWATM-SOX

Output analysis: CDTAPE

Program Corrections Decks

The following cards are used in all corrections decks and so are listed only once. For these cards and all others shown on the succeeding pages a complete explanation of their form and specification is not given. For this information consult the MACC 1180 Computing Handbook (Madison Academic Computing Center 1980) or ASCII FORTRAN Programming Manual (Sperry Rand Corporation 1979).

```
@Run,/R USERNAME,PROJNUMBER,USERID
@PASS USERPASSWORD
@ASG,AX USERPROGFILE.
@USE U,USERPROGFILE
           .
           .
           .
           .
(corrections deck)
           .
           .
           .
           .
@FIN
```

Program Corrections Decks

PLUMEPOT--

none

MODEL-EMISS--

This program is actually two separate programs (one in ASCII FORTRAN and one in UDH) but they must be run sequentially in the same job, therefore they have not been referred to separately before this. The ASCII program performs all the calculations and stores the emissions on a temporary file. The short UDH program called EMISSFILE transfers this file to a named element of a mass storage file. The reason for the second program is that ASCII can not directly write to a named element in mass storage.

```
MODEL-EMISS - none

EMISSFILE - @UDH,US U.EMISSFILE
            -4,4
            ____MODE,ELEMENT,FILENAME=USER*EMISSMET,ELTNAME=?
```

where: 'FILENAME' is the user-created emission/met data file and the 'ELTNAME' is a user-given name to the element within the file. A single run of MODEL-EMISS and EMISSFILE creates one element. A single element should contain the emissions inventory for one model run.

SFCOBSDATA--

The sole input to this program is the NCC Hourly Surface Observations tape. It is set up for handling this tape's format.

```
@UDH,US U.SFCOBSDATA
-17,17
____<STATID,EQ,?>
-21,21
____<YR,EQ,?>
```

where: STATID is the five-digit NCC station number, and YR is the two-digit year (i.e., 80 for 1980).

MIXINGHTDATA--

The sole input to this program is the NCC Twice Daily Mixing Heights tape. It is set up for handling this tape's format.

```
@UDH,US U.MIXINGHTDATA
-12,12
____<STATID,EQ,?>
-16,16
____<YR,EQ,?>
```

where: The same numbers as in the surface tape will apply here.

PRECIPDATA--

The sole input to this program is the NCC Hourly Precipitation tape. It is set up to handle this tape's format.

```
@UDH,US U.PRECIPDATA
-25,25
____<STATID,EQ,?>
-29,29
____<YR,EQ,?>
```

where: STATID will be a four-digit NCC station number different from that of the above two tapes; the year will be the same.

METDATA--

The major input to this program is the three tape files created by the above three UDH programs. Similar to the MODEL-EMISS program there are again two separate programs which must be run together.

METDATA - none

```
METFILE - @UDH,US U.METFILE
          -4,4
          ____MODE,ELEMENT,FILENAME=USER*EMISSMET,ELTNAME=?
```

where: This is the same as the EMISSFILE program. The 'FILENAME' will be the same as used before, but the 'ELTNAME' will be a different user-created name. A single run of METDATA and METFILE creates one named element in the USER*EMISSMET file. A single element contains 1-yr of meteorological data for one station.

APINFO--

This FORTRAN PROC (as explained in Section 11) contains the regional cell structure parameters which must be changed for the user's model application.

```
@PDP,FUL U.APINFO
-3,7
_______PARAMETER NUMXF=?, NUMYF=?
_______PARAMETER NUMX=?, NUMY=?, NUMZ=?
_______PARAMETER NUMS=?
_______PARAMETER MGRID=?
_______PARAMETER NUMT=?
```

where: NUMXF is number of grids in fixed system in north to south direction
NUMYF is number of grids in fixed system in west to east direction
NUMX is number of grids in rotating system in north to south direction
NUMY is number of grids in rotating system in west to east direction
NUMZ is number of cells in vertical
NUMS is number of sources (i.e., number of input emission cards)
MGRID is number of subdivisions of grid such that each grid will be subdivided into $(MGRID)^2$ subgrids for purpose of transfering concentrations back and forth between fixed and rotating systems
NUMT is number of time steps within 1 hr

UWATM-SOX--

```
@FTN,USZ U.UWATM-SOX
-859,859
 1350 FORMAT (1X,?F7.2)
```

In the FORMAT statement the "?" should be an integer value equal to the NUMYF interger. This corrects the array printout form to correspond to the user's region.

CDTAPE--

```
@FTN,USZ U.CDTAPE
-639,641
 2001 FORMAT (1X,?F7.2)
 2003 FORMAT (1X,?F7.3)
 2005 FORMAT (1X,?I7)
```

where: In all the FORMAT statements the "?" should be an integer value equal to the NUMYF interger. This corrects the array printout form to correspond to the user's region.

The Program Input Cards

PLUMEPOT--

1. Source names

```
      READ (5,111,END=20)SNAME
  111 FORMAT (A12)
```

   Example:

   ATIKOKAN____

   Comment: One card for each source.

2. Source stack data

```
      READ (*,*,END=10)HSTK,DIA,TS,GFLOW,QQ
```

   Example:

   650. 12.5 265. 610330. 77520.

   Comment: One card for each stack (may be more than one stack per source). Each point source will have one name card and one or more stack data cards. The two types are separate so the stack data can be punched in free format. The input deck will be such that the name card appears first, then cards for all the stacks for that source and then an '@EOF' card at the end of every set of cards for a given source.

   where: HSTK is stack height (ft)
   DIA is stack diameter (ft)

TS is stack gas temperature (°F)
GFLOW is stack gas-flow rate (cfm)
QQ is stack emission rate (tons/yr)

MODEL-EMISS--

Different from the PLUMEPOT deck, this deck requires a name and stack data card for each source. Again, the two are separate so the stack data can be punched in free format. The year and region cards serve only to title the printed output. The end of the complete data deck is marked with an '@EOF' card.

1. Year

```
      READ(*,*) IYEAR
```

Example:

```
1982
```

Comment: 1 card/run

2. Region name

```
      READ(5,205) REGION
  205 FORMAT (A25)
```

Example:

```
N.W. MINN - S. ONTARIO___
```

Comment: 1 card/run

3. Source names

```
      READ(5,200,END=20) SNAME
  200 FORMAT (A12)
```

Example:

```
ATIKOKAN____
```

Comment: 1 card/stack.

4. Source stack data

```
      READ(*,*)IXQ,IYQ,HSTKE,DIAE,TSE,GFLOWE,QQE
```

Example:

```
4 7 649.64 12.47 265.4 610329.6 77520.
```

Comment: 1 card/stack.

where: IXQ,IYQ are grid ID's for each source
(The E at the end of each variable symbolizes English units)
HSTKE is stack height (ft)
DIAE is stack diameter (ft)

TSE is stack gas temperature (°F)
GFLOWE is stack gas-flow rate (cfm)
QQE is stack emissions rate (tons/yr)

EMISSFILE--

no outside input cards needed

SFCOBSDATA--

none

MIXINGHTDATA--

none

PRECIPDATA--

none

METDATA--

1. File moving parameters

```
READ (*,*) MVFIL1,MVFIL2,MVFIL3
```

Example:

```
0 1 2
```

where: MVFIL1 is number of files on tape to move past to reach start of surface data
MVFIL2 is number of files on tape to move past to reach start of mixing height data
MVFIL3 is number of files on tape to move past to reach start of precipitation data

2. Latitude and longitude

```
READ(*,*)LAT,LONG,LSTD
```

Example:

```
48.57 93.38 90.
```

Comment: 1 card/run

where LAT,LONG are latitude and longitude of meteorological station (degrees)
LSTD is longitude of standard meridian for local time zone (degrees)

METFILE--

no input cards needed

APINFO--

none

UWATM-SOX--

1. Grid size, lower cell parameters

```
       READ(*,*) DX,DY,NBOXL,DZG
```

   Example:

```
30000. 30000. 3 50.
```

   where:
   DX is grid size in north-south direction
   DY is grid size in west-east direction
   NBOXL is number of lower level fixed-height cells
   DZG is fixed height of lower cells (m)

2. Pollutant species and year

```
       READ(*,*) ISP,ISPI,IYR
```

   Example:

```
1 2 1982
```

   where: ISP,ISPI are the numeric symbols for species type (1=SO_2, 2=SO_4)
   IYR is four-digit year

   Comment: 1 card/run

3. Day, month, and hour at start and end of program; how often to print concentration and mass balance information; if want to echo print meteorological data

```
      READ (5,102) IMBEG,IDBEG,IHBEG,IMSTOP,IDSTOP,IHSTOP,IPRNTV,
                   METPNT
  102 FORMAT (6I3,I10,3X,A3)
```

   Example:

```
  1  1  0 12 31 23       400   YES
```

   where: IMBEG,IDBEG,IHBEG are month, day, hour of beginning of simulation period
   IMSTOP,IDSTOP,IHSTOP are month, day, hour of end of simulation period
   (Note: This start and stop is not the same as the automatic stop/start capability. The above refers to where to begin and end calculations, the other to provide program interruption. The above allows the user to run for any selected shorter time period within the entire potential simulation period. This can be useful for testing, sensitivity analysis, special runs, etc.)

IPRNTV is the print value, every IPRNTV-th hour will be printed
METPNT is a 'Yes' or 'No' variable which indicates if the hourly input meteorological data should be echo printed

Comment: 1 card/run

4. Chemical reaction rates and surface resistances

```
      READ (*,*) R1D,R1N,RS1S,RS1W,RS2S,RS2W
```

Example:

```
2.0 .5 .5 3.0 5.0 5.0
```

where: R1D is day-time reaction rate for SO_2 to SO_4 (%/hr)
R1N is night-time reaction rate for SO_2 to SO_4 (%/hr)
RS1S is surface resistance of SO_2, summer (sec/cm)
RS1W is surface resistance of SO_2, winter (sec/cm)
RS2S is surface resistance of SO_4, summer (sec/cm)
RS2W is surface resistance of SO_4, winter (sec/cm)

Comment: 1 card/run

5. Air density, surface roughness, lateral diffusivity coefficients

```
      READ(*,*) RHOA,ZR,EDDYN,EDDYS,EDDYU
```

Example:

```
.001204  1.00  100.  100.  100.
```

where: RHOA is ambient air density (g/m^3)
ZR is surface roughness (m)
EDDYN,EDDYS,EDDYU is lateral diffusivity coefficients for neutral, stable, and unstable conditions respectively (see p. 47 for a discussion of these variables)

CDTAPE--

1. Pollutant species and year

```
      READ (*,*) ISP,ISPI,IYR
```

(This is exactly the same as for the main program.)

2. Time period to process and swap tape

```
      READ (5,20)IMB,IDB,IHB,IME,IDE,IHE,SWAPTP
   20 FORMAT(6I3,3X,A3)
```

Example:

```
  8  1  0  8 31 23    NO
```

where IMB,IDB,IHB,IME,IDE,IHE are analagous to the beginning and end of the simulation period in the main program. The CDTAPE program can perform an analysis for any sequential zone within (and up to) the entire simulation period.

SWAPTP is a 'yes' or 'no' variable which tells the program if the main program's hour-by-hour output is stored on more than 1 tape.

Comment: 1 card/run

3. Print mass balance terms

```
      READ(5,30)CMPRNT,ICMMB,ICMHB,ICMME,ICMDE,ICMHE
   30 FORMAT(A3,5X,6I5)
```

Example:

```
 NO    0     0     0     0     0     0
```

where: CRRMT is a 'yes' or 'no' variable indicating if a detailed printout of the hour-by-hour mass balance terms is to be performed.

ICMMB,ICMDB,ICMHB,ICMME,ICMDE,ICMHE indicate the month, day, hour to begin and end the detailed printout.

(Note: This operation is seldom used except for troubleshooting.)

Comment: 1 card/run

4. Number of files on tape to be processed

```
      READ(*,*)NMFILS
```

Example:

```
1
```

where NMFILS is the number of files of hour-by-hour data to process; generally it will be only one.

Comment: 1 card/run

5. Grids for which to calculate concentration frequency distribution

```
     READ(*,*)NPTS
     READ(*,*)(IX(I),I=1,NPTS)
     READ(*,*)(IY(I),I=1,NPTS)
```

Example:

```
5

9 6 8 2 2

2 4 8 5 10
```

where: NPTS is the number of grids for which the frequency table is
to be calculated and printed.
IX,IY are the grid ID's of the above points.

SUMMARY

In summary, a suggested procedure for program preparation is:

1. Create USER*PROGFILE
2. Create USER*EMISSMET
3. Create USER*STOPSTART
4. Obtain tape for intermediate meterololgical-data processing
5. Obtain tapes for UWATM-SOX hourly output
6. Construct and execute corrections decks
7. Construct data-decks

Once these seven steps are complete the entire sequence of model programs will be ready for execution.

SECTION 13

PROGRAM EXECUTION

This and the previous sections describe everything the user needs to operate the programs. The previous section discussed how to prepare them for execution by making internal program changes through the corrections decks and constructing the input data cards required for the run-decks to be discussed in this section. This section explains for each program:

1. Run-deck construction
2. Output mode and format

The run-deck includes all cards which must be typed and submitted as a unit to execute one program. The output mode (tape, mass storage, line-printer) and exact format of the output are given for each executed program.

The form of the discussion is similar to the previous section in that first the run-decks for each and every program are described, and then the output mode and format for each and every program is described.

The form of the run-deck discussion will be as follows. First, the general run-cards which are required for all run-decks are listed. Next, the run deck for each program is listed together with the input data card examples in the previous section. If the user executes one program more than once then of all the run-deck cards only the data cards will need to be changed. The remaining cards of the run deck remain the same from run to run. After the listing, any relevant comments concerning the execution procedure will be given. The run-deck for each program need only be combined with the general run cards for the user to be ready to execute.

The form of the output discussion will be as follows. First, the WRITE or PRINT statement(s) are listed together with the associated FORMAT statement(s). This listing serves to acquaint the user with actual output device specification and format spacing on that device as they appear in the computer code. Next, the output variables are defined and their units given. Finally, any comments relevant to the output are given. Not all the output statements are listed because for some programs it would be too cumbersome and not very instructive. Therefore, only the outputs essential to the continuous flow of operation of the program are given. The analysis of the final model output is discussed in the next section.

SEQUENCE OF PROGRAM DISCUSSION

Emissions: PLUMEPOT
MODEL-EMISS

Met data: SFCOBSDATA
MIXINGHTDATA
PRECIPDATA
METDATA

Main Program: INITSPST
UWATM-SOX

Output Analysis: CDTAPE

PROGRAM RUN-DECKS

The following cards will be used with all run decks and therefore are only listed this once. For complete details of each card's specification consult the MACC 1180 Handbook (Sperry Rand Corporation 1979) or ASCII FORTRAN Programming Manual (Madison Academic Computing Center 1980).

```
@RUN,/R USERNAME,PROJNUMBER,USERID,COST/TIMELIMIT
@PASS USERPASSWORD
@ASG,AX USERPROGFILE.
@USE U,USERPROGFILE
            .
            .
            .
            .
    (run deck)
            .
            .
            .
            .
@FIN
```

PLUMEPOT

```
@PRT,S U.PLUMEPOT
@MAP,IS
__IN U.PLUMEPOT
__LIB FTN*LIB.
@XQT
ATIKOKAN
650._12.5_265._610330._77520.
@EOF
```

MODEL-EMISS

```
@ASG,AX USER*EMISSMET.
@USE D,USER*EMISSMET
@ASG,T 11.
@PRT,S U.MODEL-EMISS
@MAP,IS
```

```
__IN U.MODEL-EMISS
__LIB FTN*LIB.
@XQT
1982
N.E._MINN_-_S._ONTARIO
ATIKOKAN
4_7_649.64_12.47_265.5_610329.6_77520.
@EOF
@PRT,S U.EMISSFILE
@MAP,IS
__IN U.EMISSFILE
@XQT
@PRT,T D.
```

Comment: The user-created USER*EMISSMET file, which stores all the necessary emissions and meterological data, has been assigned to the run. First MODEL-EMISS is executed, then the EMISSFILE program. EMISSFILE stores the processed emissions data as a named element on the USER*EMISSMET file. The element name is given in the EMISSFILE program. Caution--each time a new element is to be added to the file the EMISSFILE program must be updated (via the corrections deck) to name the new element.

SFCOBSDATA

```
@ASG,TV_NOAA.,U9V////FLDATA/EBCDIC/6,xxxxxx
@ASG,TVF_10.,U9V,$uuuuuu
@REELID_uuuuuu/tapelabel
@MOVE 10.,n
@PRT,S U.SFCOBSDATA
@MAP,IN
__IN U.SFCOBSDATA
@XQT
```

Comment: The 'xxxxxx' is the reel identification number to be user-supplied for the NCC Surface Observations tape. The 'uuuuuu' is the reel ID for the user's meteorological data tape. This tape is assumed to have a tape label for protection purposes. First the NCC tape is hardware translated, then SFCOBSDATA processes the data and outputs it onto a tape file whose position is indicated by the @MOVE statement. It will be file number n+1. The @MOVE statement dictates moving past n files and positioning itself at the head of file n+1 which is to be written.

MIXINGHTDATA

```
@ASG,TV_NOAA.,U9V////FLDATA/EBCDIC/6,yyyyyy
@ASG,TVF_10.,U9V,$uuuuuu
@REELID_uuuuuu/tapelabel
@MOVE 10.,n
```

```
@PRT,S U.MIXINGHTDATA
@MAP,IN
__IN U.MIXINGHTDATA
@XQT
```

Comment: The 'yyyyyy' is the reel ID for the NCC Twice Daily Mixing Heights tape. The user's meteorological data tape reel ID and tape label are the same as above. First the NCC tape is hardware translated then MIXINGHTDATA processes the data and outputs it onto a tape file whose position is indicated by the @MOVE statement.

PRECIPDATA

```
@ASG,TV_NOAA.,U9V////FLDATA/EBCDIC/6,zzzzzz
@ASG,TVF_10.,U9V,$uuuuuu
@REELID_uuuuuu/tapelabel
@MOVE 10.,n
@PRT,S U.PRECIPDATA
@MAP,IS
__IN U.PRECIPDATA
@XQT
```

Comment: The 'zzzzzz' is the reel ID for the NCC Hourly Precipitation Data tape. The user's meteorological data tape reel ID and tape label are the same as above. First, the NCC tape is hardware translated, then the PRECIPDATA processes the data and outputs it onto a tape file whose position is indicated by the @MOVE statement.

METDATA

```
@ASG,TVF_10.,U9V,$uuuuuu
@REELID_uuuuuu/tapelabel
@ASG,AX_USER*EMISSMET.
@USE D,USER*EMISSMET
@ASG,T 11.
@PRT,S U.METDATA
@MAP,ISE
__IN U.ASCIIMATRIX
__IN U.METDATA
__IN A
__IN B
__LIB FTN*LIB.
@XQT
0_1_2
47.57_93.38_90.
@PRT,S U.METFILE
@MAP,IS
__IN U.METFILE
@XQT
@PRT,T D.
```

Comment: The three previously created UDH tape files on tape 10 are used by the METDATA program to create a single 1 yr file of all the meteorological data which is temporarily written on file 11. The UDH program METFILE transfers file 11 to the USER*EMISSMET file under the element name given in METFILE. Caution--each time a new meteorological element is to be added to USER*EMISSMET the METFILE program must be updated (through the corrections deck) to name the new element.

INITSPST

```
@ASG,AX_USER*STOPSTART.
@USE 9,USER*STOPSTART
@PRT,S U.INITSPST
@MAP,IS
__IN U.INITSPST
__LIB FTN*LIB.
@XQT
```

Comment: Before every new run of the main program UWATM-SOX the stop-start file must be zeroed. The user must create a separate file for this purpose and it must be given the number 9 in the @USE statement.

UWATM-SOX

```
@ASG,AX USER*EMISSMET.
@USE D,USER*EMISSMET
@ASG,AX_USER*STOPSTART
@USE_9,USER*STOPSTART
@ASG,TVF_20.,U9V,$aaaaaa
@REELID_aaaaaa/tapelabel
@ASG,T 21.,F
@ASG,T 23.,F
@PRT,S U.APINFO
@PRT,S U.UWATM-SOX
@MAP,ISE
__IN_U.UWATM-SOX
__IN_U.ASCIIMATRIX
__IN_U.WINDIF-PRFLS,.PLUME-RISE,.DEP-VEL,.WET-DEP
__IN_U.E-TFM, .RF-TFM, .FR-TFM
__IN_HUGE
__IN_BIG
__LIB_FTN*LIB.
@XQT
1_2_1982
__1__1__0_12_31_23_______400___YES
2.0_.5_.5_3.0_5.0_5.0
@ADD D.E-eltname
@ADD D.M-eltname
```

Comment: Tape 20 is a user-supplied tape containing the hourly output. It is assumed to be tape labeled for protection purposes. The input deck consists of five cards, three data cards and two @ADD cards which bring in the necessary emissions and meteorological data. 'E-eltname' is the emissions data element name given in EMISSFILE and 'M-eltname' is the meteorological-data element name given in METFILE.

CDTAPE

```
@ASG,TVF_20.U9V,$aaaaaa
@REELID_aaaaaa/tapelabel
@PRT,S U.CDTAPE
@MAP,IS
__IN U.CDTAPE
__IN U.ISLOT
__LIB FTN*LIB.
@XQT
1_2_1982
__8__1__0__8_31_23____NO
_NO_________0____0____0____-0____0
1
5
9_6_8_2_2
2_4_8_5_10
```

Comment: none

PROGRAM OUTPUT

PLUMEPOT

```
______PRINT 201,HSTK,DIA,TS,GFLOW,QQ,POT
  201_FORMAT(17X, F6.0, 4X, F5.1, 4X, F9.0, 4X, F10.0, 4X, F8.0, 4X,
          F15.3)
where HSTK is stack height (ft)
       DIA is stack diameter (ft)
        TS is stack gas temperature (°F)
     GFLOW is stack gas-flow rate (cfm)
        QQ is stack emissions rate (tons/yr)
       POT is plume rise potential
```

Comment: The output is line printed only.

MODEL-EMISS

```
______WRITE(11,211)SNAME, IXQ, IYQ, HSTK, DIA, TS, GFLOW, QQ
__211_FORMAT(A12, 2X, I3, 2X, I3, 2X, F4.0, 2X, F3.1, 2X F5.0, 2X, F5.0,
          2X, F5.0)
where SNAME is the point source name
        IXQ is north-south direction grid ID
        IYQ is west-east direction grid ID
```

HSTK is stack height (m)
DIA is stack diameter (m)
TS is stack gas temperature (°K)
GFLOW is stack gas-flow rate (m^3/sec)
QQ is stack emissions rate (g/sec)

Comment: The above output is written onto a temporary file 11, the UDH EMISSFILE program then places it into USER*EMISSMET under the user-supplied element name. The above output is also line printed but the PRINT statements have not been shown.

SFCOBSDATA

```
_OUTPUT, SFCYR
___MODE, SDFTAPE, FILENAME=10
```

Comment: The entire 1 yr of data is written onto tape 10 as one file. The format of each record (hr) within the file (yr) is 37 characters long as follows:

```
YR__MN__DY__HR__CEIL__WD__WS__TMP__CC
```

where: YR is year (00-99)
MN is month (01-12)
DY is day (01-31)
HR is hour (00-23)
CEIL is ceiling height (000-990 100's of ft)
WD is wind direction (00-36, terms of degrees clockwise from north)
WS is wind speed (00-99 knots)
TMP is dry bulb surface temperature (0-199, whole day °F)
CC is cloud cover (0-9, tenths of total sky covered)

The input format in the METDATA program to read each record is:

```
FORMAT (I2,2X,I2,2X,I2,2X,I2,2X,I4,2X,I2,2X,I2,2X,I3,2X,I2)
```

MIXINGHTDATA

```
_OUTPUT, ZMYR
___MODE, SDFTAPE, FILENAME=10
```

Comment: The entire 1 yr mixing height data is written onto tape 10 as one file. The format of each record (day) within the file (yr) is 16 characters long as follows:

```
YR__MN__DY__ZMAF
```

where: YR,MN,DY are the same as above
ZMAF is afternoon mixing height (000-9999 m above ground)

The input METDATA format to read each record is:

```
FORMAT (I2,2X,I2,2X,I2,2X,F4.0)
```

PRECIPDATA

```
_OUTPUT, PRECIPYR
___MODE, SDFTAPE, FILENAME=10
```

Comment: The entire year's worth of precipitation data is written onto tape 10 as one file. The format for each record (day in which precipitation occured) within the file (yr) is 124 characters long as follows:

```
YR__MN__DY__H01_H02_H03_...._H23_H24____DTOT____MTOT
```

where: YR,MN,DY are the same as above
H01-H24 are the total precipitation for each hour of the day (1/100's of inches, H01 corresponds to 00-01 local standard time, H02 to 01-02 LST, etc.)
DTOT is total of the day
MTOT is total of the month

The METDATA input format is:
FORMAT (I2,2X,I2,2X,I2,2X,24(I3,IX))
Note: The DTOT and MTOT are not read into the program

METDATA

```
______WRITE(11,700) JMON(I), JDAY(I), JHR(I), IDIR(I), IUS(I), ISTAB(I),
                    IHFLUX(I), ITA(I), ZMHR(I), IRAIN(I), ISNOW(I),
                    I=1, NDATA)
__700_FORMAT
        (1X,I2,2X,I2,2X,I2,4X,I3,2X,I3,2X,I1,2X,I3,2X,I3,4X,I4,
        4X,I3,2X,I3)
```

where: JMON is month (01-12)
JDAY is day (01-31)
JHR is hour (00-23)
IDIR is wind direction (degrees clockwise from north)
IUS is wind speed ((m/sec)*10)
ISTAB is stability class (1-7)
IHFLUX is heat flux values (($cal/cm^2/sec$)*100)
ITA is surface air temperature (°K)
ZMHR is mixing height (m)
IRAIN is rainfall (1/100ths of inches)
ISNOW is snowfall (1/100ths of inches water equivalent)
NDATA is number of hours in year (8760 or 8784)

Comment: The above hourly METFILE output for 1 yr is written onto temporary file 11, the UDH program then places it into the USER*EMISSMET file under the user-supplied element name. The data is also line printed but the PRINT statements are not shown here.

INITSPST

Comment: This program zeros the stop-start flag (ISPST) in the USER*STOPSTART file, which indicates to the main program if the current run is new or a restarted run.

UWATM-SOX

```
______IF(IRAIN.EQ.0.AND.ISNOW.EQ.0) THEN
______CALL FLK$6(IOTPOT,20,1,APINFO,KAPWD,$950,$960)
ELSE
      CALL FLK$6(IOTPOT,20,1,APINFO,KAP  ,$950,$960)
END IF
```

Comment: All hourly information to be written on tape 20 is stored in the single-dimensioned APINFO array. The decomposition of this array is given in the APINFO FORTRAN PROC. Extensive hourly data is line printed periodically according to the value specified on the second data card above. This printout is not discussed here.

CDTAPE

Comment: A sample of the line printer output is shown in the next section. The PRINT statements are not separately given as there are many and it would not be instructive to list them all. The analyzed output is discussed in the next section.

SECTION 14

OUTPUT ANALYSIS

This section describes the final model products. It describes:

1. The CDTAPE program's hour-by-hour analysis
2. The isopleth computer plots

Each is discussed briefly.

CDTAPE ANALYSIS

The CDTAPE (Concentration-Deposition Tape Processor) analyzes the UWATM-SOX program's hour-by-hour output stored on tape. The types of results which are currently available are listed in Table 8 but are not the only ones possible. An example of some of the types of results are given in Figures 13 to 17. The methods by which the CDTAPE results are obtained is not discussed. Though they are relatively simple conceptually, they involve considerable programming detail.

COMPUTER PLOTS

It is assumed that users will have access to their own computer plotting facilities, therefore the plotting routines used in our modeling work are not discussed except to say we use the WISMAP2 plotting package developed by the University of Wisconsin-Madison Cartography Laboratory. Users may, if they wish, use this package. To do so contact:

Howard Meade
c/o Cartographic Lababoratory
464 Science Hall
University of Wisconsin-Madison
Madison, WI 53706
(608) 262-1363

An example of a isopleth computer map is given in Figure 18.

SUMMARY

Table 8 lists all model outputs currently available from the UWATM-SOX, CDTAPE and computer plotting programs. It distinguishes the spatial and temporal resolution and type of output. A representative sample of some of the outputs is given in Figures 13 through 18.

TABLE 8. SUMMARY OF MODEL OUTPUT

Resolution		
Spatial	Temporal	Output type
Region	Hourly	UWATM-SOX outputs: Date Met data values Wind-diffusivity profiles Plume data Regional mass balance information Ground level concentrations (SO_2 and SO_4) Dry deposition (SO_2 and SO_4) Wet deposition (SO_2 and SO_4)
Ground level regional grid array	Annual average	Concentration (SO_2 and SO_4)
Ground level regional grid array	Total annual	Dry deposition (SO_2 and SO_4)
Ground level regional grid array	Total annual	Wet deposition (SO_2 and SO_4)
Ground level regional grid array	Total seasonal	Dry deposition (SO_2 and SO_4)
Ground level regional grid array	Total seasonal	Wet deposition (SO_2 and SO_4)
Ground level regional grid array	Total annual	Wet + dry deposition (SO_2, SO_4, combined as SO_4)
Ground level regional grid array	Maximum 24-hr	Concentration and date (SO_2 and SO_4)
Ground level regional grid array	Maximum 3-hr	Concentration and date (SO_2 and SO_4)
Ground level regional grid array	Hourly	pH of precipitation (output from WETDEP subroutine)
Per selected grid	1-hr	Annual and seasonal frequency distribution of ground level concentrations (SO_2 and SO_4)
Per selected grid	3-hr	Annual and seasonal frequency distribution of ground level concentrations (SO_2 and SO_4)
Per selected grid	24-hr	Annual and seasonal frequency distribution of ground level concentrations (SO_2 and SO_4)
Region	Annual	Total SO_2/SO_4 budget from in-region sources
Region	Annual seasonal	Computer isopleth plots (SO_2, SO_4, and combined)

```
*** ANNUAL AVERAGE GROUND LEVEL CONCENTRATION FOR   SO2   (MICROGRAMS/METER**3) ***

 -------------------------------------------------------------------------------------
        .05     .08     .09     .17     .31     .32     .48     .39     .15     .25     .16
        .07     .09     .13     .15     .32     .36     .61     .41     .41     .36     .27
        .08     .04     .12     .16     .27    1.05    1.23     .58     .60     .25     .38
        .07     .10     .12     .23     .42     .38    4.56    1.77     .71     .48     .33
        .06     .08     .16     .22     .40     .44     .80    1.21     .84     .46     .29
        .09     .13     .19     .20     .23     .49     .29     .45     .69     .41     .43
        .05     .19     .07     .09     .27     .26     .30     .26     .17     .59     .20
        .08     .09     .17     .17     .12     .21     .18     .19     .27     .18     .17
        .06     .09     .14     .12     .13     .11     .15     .17     .21     .16     .10
        .07     .08     .09     .11     .12     .08     .16     .16     .11     .13     .13
        .07     .02     .09     .06     .08     .12     .12     .10     .11     .05     .10
        .06     .08     .06     .05     .06     .06     .08     .08     .09     .10     .08
        .04     .06     .03     .05     .05     .06     .07     .08     .07     .06     .05

 -------------------------------------------------------------------------------------
*** TOTAL ANNUAL DEPOSITION (WET + DRY) FOR   SO2   (KILOGRAMS/HECTARE) ***

 -------------------------------------------------------------------------------------
       .160    .244    .299    .587   1.088   1.054   1.463   1.227    .430    .640    .365
       .186    .301    .439    .506   1.092   1.257   1.950   1.332   1.085    .819    .573
       .219    .105    .356    .541    .898   3.837   4.032   1.622   1.517    .628    .848
       .185    .278    .344    .641   1.242   1.2[illegible]8  14.585   4.679   1.720   1.068    .738
       .149    .217    .411    .599   1.115   1.30[illegible]   2.566   3.281   2.075   1.104    .666
       .186    .294    .446    .541    .687   1.475    .891   1.306   1.713    .964    .964
       .131    .442    .202    .238    .757    .744    .854    .757    .471   1.381    .439
       .163    .245    .457    .458    .357    .593    .497    .541    .719    .473    .401
       .140    .250    .352    .334    .391    .296    .394    .488    .565    .409    .257
       .171    .215    .253    .308    .345    .208    .418    .419    .294    .350    .312
       .194    .058    .255    .175    .237    .338    .333    .267    .285    .136    .270
       .137    .203    .171    .147    .163    .155    .230    .208    .222    .238    .195
       .100    .150    .081    .147    .144    .169    .190    .203    .172    .151    .127
```

Figure 13. Example of ground level concentration and deposition arrays.

```
*** MAXIMUM 24 HOUR CONCENTRATION FOR    SO2   (MICROGRAMS/METER**3) ***

----------------------------------------------------------------------------------------
      3.52    3.69    3.88    5.55    4.77    3.82    8.34    7.97    2.87    4.21    3.13
      2.96    3.17    4.33    4.03    5.53    4.20    8.13    8.20    6.58    5.63    4.95
      2.47    1.31    2.91    3.14    5.32   10.73   15.92    7.31    6.78    4.54    4.89
      2.37    3.18    3.02    6.22    6.25    5.96   17.42   13.99    7.13    7.45    5.56
      2.18    2.43    3.17    4.70    7.77    6.76    8.90    8.66    7.79    4.05    4.28
      3.00    3.35    5.39    4.89    4.41    6.89    3.31    5.53    6.40    4.18    6.27
      1.34    9.04    1.47    1.33    4.82    5.10    5.86    5.32    2.56    9.27    3.64
      3.66    1.90    2.74    3.85    2.17    4.81    2.63    3.91    4.50    1.95    2.70
      1.73    2.12    5.34    2.03    3.35    3.12    3.05    3.40    4.02    2.51    1.17
      2.31    2.10    1.75    2.22    2.92    2.08    4.04    3.81    2.99    2.34    2.11
      1.92     .59    2.06    1.75    2.49    2.59    3.11    2.46    2.44    1.09    2.63
      1.74    2.09    1.78    2.05    1.67    1.65    1.86    2.77    2.00    2.45    1.88
      1.11    1.57    1.12    1.83    1.92    1.46    2.06    3.29    1.83    1.57    1.31

----------------------------------------------------------------------------------------
*** MAXIMUM  3 HOUR CONCENTRATION FOR    SO2   (MICROGRAMS/METER**3) ***

----------------------------------------------------------------------------------------
     10.52   11.23   10.94   17.05   19.09   14.84   14.68   24.11    6.97   10.67    7.48
      7.49    7.83   11.63   11.89   20.57   19.18   16.53   23.86   14.77   15.91   12.47
      7.77    6.18    8.27   11.47   19.85   49.01   46.84   23.29   28.14   13.40   21.30
      6.54    7.08   10.80   15.67   14.22   15.94   72.79   45.80   19.19   16.28   12.74
      5.46    5.84   16.23   12.68   23.82   22.60   20.73   24.16   17.37   13.36    8.57
     13.41   10.54   19.93   16.78   16.74   17.83   10.33   14.37   17.29    9.03   13.26
      4.61   45.11    5.46    5.83   13.22   12.51   12.68    9.31    7.70   13.76    9.04
     17.99    6.23    7.24   10.30    6.07   10.38    7.93    8.69    9.18    6.73    7.16
      6.19    8.30   14.40    7.18    5.97    6.78    8.39    8.67    9.46    7.08    4.69
      7.96    7.09    5.45    7.69    5.50    4.61    7.57   11.37    6.68    6.07    6.17
      7.01    2.21    4.87    6.13    7.76    5.83    7.73    9.36    4.58    3.92    9.65
      6.31    5.49    3.33    3.17    4.19    3.95    5.66    7.48    6.78    5.31    4.72
      2.89    4.44    2.49    3.02    3.82    3.62    5.33    6.93    4.25    3.79    2.80
```

Figure 14. Example of maximum 24- and 3-hr concentration arrays.

```
DATES OF 3-HR AND 24-HR MAXIMUMS
     (NOTE - ALL DATES ARE CALCULATED AS FOLLOWS, DATE = MONTH*100 + DAY, SO FEB 12=212, DEC 25=1225)

24-HR MAXIMUMS FOR   SO2   ***

   123    123    110    110   1203    118    105   1117   1116   1114   1116
   123    123    123    123    110   1203    105   1117   1114    206    206
   124    320    326    326    123   1203    105   1114   1115    108    108
  1210   1210    124    416    312    417   1208   1208   1208   1208   1208
  1210    416    312   1209    312    312   1230    222    103    103   1208
  1209    302    312    312    312    421    312    305   1107    221    103
   309    312    407    423    312    421   1230    305    222   1112   1112
   312    309    312    312    422    421   1030    305    305   1230   1112
   309    312    312    422    422    421   1230    305    305    122    122
   312    312    426    422    421    421   1230    305   1230   1121    122
   312    421    422    421    421    421   1230    305   1121   1110   1121
   312    426    422    422    421    421   1230   1230   1230   1121   1121
   426    422    422    422    421    421   1230   1230   1121   1121   1121

3-HR MAXIMUMS FOR   SO2   ***

   122    122    110    129    912   1213   1118   1116    324    202   1115
   122    122    122    122    912    915    127   1116   1114   1117   1115
   124    123    122    122    823    917    104   1027    202   1207   1207
   416    319    416    416    311    712   1207   1207   1207   1207    116
   319    416    311    423    311    311    427    812    326   1212   1208
   311   1209    311    311    427    427   1029   1230    116    221   1212
   311    311    423    423    427   1229   1230   1122    221    812    103
   311    311    311    426    427   1229   1029    304    304   1220   1111
   311    403    312    426    421    421   1229    629    304   1220   1217
   311    426    426    622    421    305   1229    305   1230   1121   1107
   426    312    426    421   1229    203   1001    203   1121   1110   1121
   426    411    421    421    421    305    305    305    203    130   1121
   426    426    421    421    421    305    305    305   1121    203   1121
```

Figure 15. Example of date arrays for 24- and 3-hr maximums.

```
FREQUENCY DISTRIBUTION TABLE FOR 1-HR, 3-HR, 24-HR AVERAGE CONCENTRATIONS FOR SELECTED GRIDS
                    ********* X =    9     Y =     2 *********

***** ANNUAL *****
                    *****  1 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   5.00  10.00  15.00  20.00  25.00  30.00  35.00  40.00  45.00  50.00 999.99
   8536    238      9      1      0      0      0      0      0      0      0      0

                    *****  3 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   5.00  10.00  15.00  20.00  25.00  30.00  35.00  40.00  45.00  50.00 999.99
   2850     76      2      0      0      0      0      0      0      0      0      0

                    ***** 24 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00 999.99
    359      8      0      0      0      0      0      0      0      0      0      0      0      0

***** SUMMER *****
                    *****  1 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   5.00  10.00  15.00  20.00  25.00  30.00  35.00  40.00  45.00  50.00 999.99
   4329     85      2      0      0      0      0      0      0      0      0      0

                    *****  3 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   5.00  10.00  15.00  20.00  25.00  30.00  35.00  40.00  45.00  50.00 999.99
   1446     26      0      0      0      0      0      0      0      0      0      0

                    ***** 24 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00 999.99
    183      1      0      0      0      0      0      0      0      0      0      0      0      0

***** WINTER *****
                    *****  1 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   5.00  10.00  15.00  20.00  25.00  30.00  35.00  40.00  45.00  50.00 999.99
   4207    153      7      1      0      0      0      0      0      0      0      0

                    *****  3 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   5.00  10.00  15.00  20.00  25.00  30.00  35.00  40.00  45.00  50.00 999.99
   1404     50      2      0      0      0      0      0      0      0      0      0

                    ***** 24 HR AVERAGES FOR  SO2      (MICROGRAMS/METER**3) *****
   1.00   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00 999.99
    176      7      0      0      0      0      0      0      0      0      0      0      0      0
```

Figure 16. Example of frequency distribution printout for one grid.

```
-------------------------------
  TOTAL MASS BALANCE FOR REGION
-------------------------------

PROCESS                                   TOTAL (GRAMS)  TOTAL (X10E9 GMS)    % OF INPUT
-------                                   -------------  -----------------    ----------

EMISSIONS INPUT                           70515927040.       70,516              *         FOR SO2

WIND BLOWN OUT                            12661650176.       12,662             18,0       FOR SO2
DRY DEPOSITION                             9981803648.        9,982             14,2       FOR SO2
WET DEPOSITION                              416873020.         ,417               ,6       FOR SO2
CHEMICAL REACTIONS (LOST)                  4742483392.        4,742              6,7       FOR SO2
GRID ROTATION SCHEME                      42683793920.       42,684             60,5       FOR SO2
LEFT IN REGION AT LAST HOUR                  29018004.         ,029               ,0       FOR SO2
DIFF. BETWEEN INPUT AND OUTPUT                 714569.         ,001               ,0       FOR SO2
    (IDEALLY = 0)                                                             ------
                                                                               100,0

EMISSIONS INPUT                            2115503952.        2.116              *         FOR SO4
CHEMICAL REACTIONS (GAINED)                7113721152.        7.114              *         FOR SO4
TOTAL INPUT (EMISS + CHEM)                 9229225088.        9.229              *         FOR SO4

WIND BLOWN OUT                             1892668432.        1.893             20.5       FOR SO4
DRY DEPOSITION                              343148512.         .343              3.7       FOR SO4
WET DEPOSITION                              308699676.         .309              3.3       FOR SO4
GRID ROTATION SCHEME                       6683304128.        6.683             72.4       FOR SO4
LEFT IN REGION AT LAST HOUR                   1362533.         .001               .0       FOR SO4
DIFF. BETWEEN INPUT AND OUTPUT                  41687.         .000               .0       FOR SO4
    (IDEALLY = 0)                                                             ------
                                                                               100.0

/////////////////////////////////////////////////////////////////////////////////////////////

TOTAL SULFUR INPUT TO REGION AS SO2       71926262784.       71.926              *

TOTAL DEPOSITED IN REGION AS SO2          10833241984.       10.833             15.1
(DRY + WET DEPOSITION)

TOTAL LEAVING REGION AS SO2               61062758400.       61.063             84.9
(WIND + ROTATION SCHEME)

TOTAL STILL IN REGION AT LAST HOUR AS SO2    29926359.         .030               .0
                                                                              ------
                                                                               100.0
```

Figure 17. Example of total regional SO_2 and SO_4 budget.

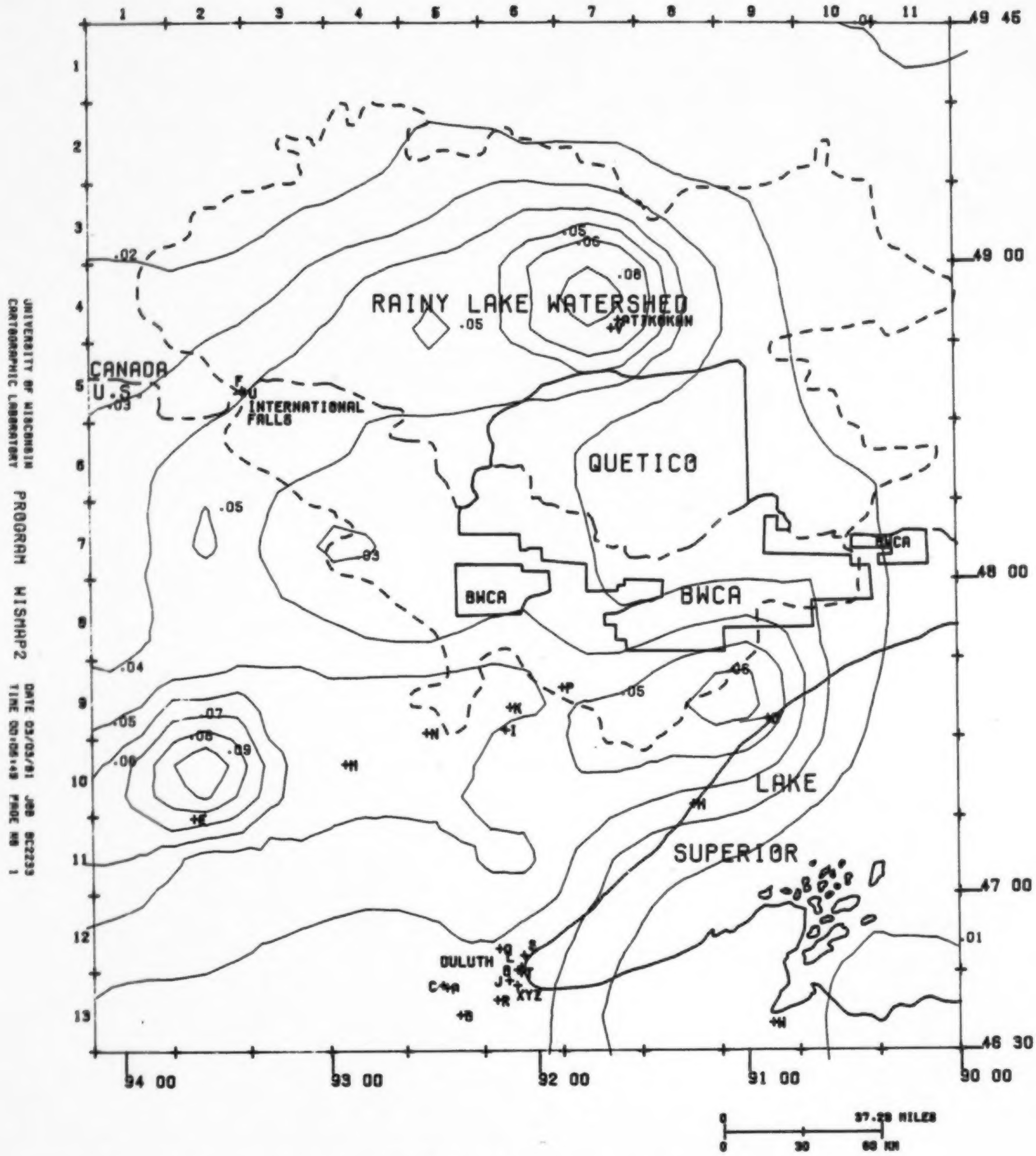

UNIVERSITY OF WISCONSIN
CARTOGRAPHIC LABORATORY
PROGRAM WISMAP2
DATE 03/03/81 JOB 8C2239
TIME 00:05:49 PAGE NO 1
RAINY LAKE WATERSHED
ATIKOKAN
CANADA
U.S.
INTERNATIONAL FALLS
QUETICO
BWCA
BWCA
BWCA
LAKE
SUPERIOR
DULUTH
.02
.03
.04
.05
.06
.07
.08
.09
.01
49 45
49 00
48 00
47 00
46 30
94 00
93 00
92 00
91 00
90 00
37.28 MILES
0
30
60 KM

Figure 18. Example of isopleth computer plot (of bulk deposition SO_2 for Atikokan Power Plant in Southern Ontario).

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APPENDIX A

EMISSIONS INVENTORY DATA SHEETS

Year: ________________ Region: ______________________________

NAME	Sub-unit #	UTM		HT. (ft)	DIA. (ft)	TEMP. (^{o}F)	FLOW (cmf)	EMISS (tons/yr)
		Horiz.	Vert.					

Figure A-1. Selected sources list.

Year: ____________ Region: ______________________________

NAME	ALTERATION

Figure A-2. Original inventory alterations record.

Year:

Region:

CHANGES	
NAME	

Figure A-3. Combined inventory alterations record.

Year:

Region:

Model Name	Grid Coord		HSTK (ft)	DIA (ft)	TS (°F)	GFLOW (cfm)	QQ (tons/yr)
	IXQ	IYQ					

Figure A-4. Comtined sources list.

APPENDIX B

SUMMARY OF USER-SUPPLIED INPUT VARIABLES

TABLE B-1. SUMMARY OF ALL USER-SUPPLIED MODEL INPUT VARIABLES

Process and program	Variable Name	Variable description	Source	Comments
Cell structure specification	NUMXF	No. of grids in fixed system	User-supplied	-See Section 12
	NUMYF			
APINFO	NUMX	No. of grids in rotating system		
	NUMY			
	NUMZ	No. of grids in vertical		
	MGRID	Grid subdivision parameter		
UWATM-SOX	DX	Grid size (m)		
	DY			
	NBOXL	No. of lower level fixed-height cells		
	DZG	Fixed height of lower cells (m)		
Time specification APINFO	NUMT	No. of time-steps per hour	User-supplied	
	IMBEG	Month, day, hour to begin simulation		
	IDBEG			
	IHBEG			
	IMSTOP	Month, day, hour to stop simulation		
	IDSTOP			
	IHSTOP			
Emissions (point sources) MODEL-EMISS	SNAME	Source name	Outside agency emissions inventories	-The source locations can be found from the inventories but the grid ID assignment must be made by hand following the grid scheme outlined in Section 12.
	IXQ	Grid ID		
	IYQ			
	HSTKE	Stack height (ft)		
	DIAE	Stack diameter (ft)		
	TSE	Stack gas temperature (°F)		
	GFLOWE	Stack gas-flow rate (cfm)		
	QQE	Stack emissions rate (tons/yr)		-The MODEL EMISS program converts all units to metric and stores the inventory on a mass storage file. UWATM-SOX inputs this file.

(continued)

Table B-1 (continued)

Process and program	Variable Name	Variable description	Source	Comments
Meteorology program SFCOBSDATA	STATID	NCC station ID	NCC surface obsservation tape	-The SFCOBSDATA program stores all hourly data as a file on a user-supplied tape.
	YR	Year		
	MON	Month		
	DAY	Day		
	HR	Hour		
	CEIL	Hourly ceiling height (100's ft)		
	WD	Hourly wind direction (10's deg)		
	WS	Hourly wind speed (knots) clockwise from north		
	TEMP	Hourly air temperature (°F)		
	CLOUD	Hourly cloud cover (1110's)		
MIXINGHTDATA	ZMAFT	Afternoon (1400) mixing height (m)	NCC twice daily mixing height tape	-The MIXINGHTDATA program stores the daily values as file on a user-supplied tape.
PRECIPDATA	---	Hourly precipitation (1/100's in.)	NCC hourly precipitation tape	-The PRECIPDATA program stores the hourly values as a file on a user-supplied tape.
METDATA	LAT	Latitude of meteorological station (°)	NCC	-Besides these three variables the METDATA program inputs the above three UDH-created files and outputs as a file on mass storage all hourly meteorological data. UWATM-SOX inputs this file.
	LONG	Longitude of meteorological station (°)		
	LSTD	Longitude of standard meridian for wind time zone		
Chemical reactions UWATM-SOX	RID	Day-time reaction rate constant (%/hr)	User-supplied	-See Section 12.
	RIN	Night-time reaction rate constant		
Removal UWATM-SOX	RS1S	Summer, winter SO_2 surface resistance (sec/cm)	User-supplied	-See Section 13.
	RS1W			
	RS2S	Summer, winter SO_2 surface resistance (sec/cm)		
	RS2W			